Tables of Molecular Vibrational Frequencies

Part 9

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Fundamental vibrational frequencies of 109 molecular forms of 38 polyatomic chain molecules consisting of the CH_3, CD_3, CH_2, CD_2, CHD, O, and S groups are given as an extension of tables of molecular vibrational frequencies published in the NSRDS-NBS publication series and in this journal. On preparing the tables in this part, an approach, different from that in the previous parts, based on the calculations of normal vibration frequencies was adopted. A set of force constants which explains all the frequencies of small molecules for which the assignments had been established was obtained and then the frequencies of larger molecules were calculated and compared with the frequencies observed in the infrared and Raman spectra. The tables provide a convenient source of information for those who require vibrational energy levels and related properties in molecular spectroscopy, thermodynamics, analytical chemistry, and other fields of physics and chemistry.

Key words: Force constants; fundamental frequencies; infrared spectra; normal vibrations; polyatomic molecules; Raman spectra; vibrational frequencies.

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1. Introduction

Establishing the assignment of molecular vibrational frequencies[1] has fundamental importance in elucidating various problems in physics and chemistry. The information concerning the force field and the motion of atoms in a molecule can be most directly derived from its vibrational frequencies. If all the vibrational frequencies of a molecule are known as well as the molecular structure, thermodynamic quantities can be easily computed on the ideal gas model. Thus the need for a tabulation of evaluated reference data on molecular vibrational frequencies has often been felt by many investigators.

In 1964 a project for producing such tables was initiated at the University of Tokyo in cooperation with the National Standard Reference Data System of the National Bureau of Standards. The evaluated data resulting from this project have been published as Tables of Molecular Vibrational Fre-

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[1] Following common usage, the term "vibrational frequencies" is used in this series, even though numerical values are given for the equivalent wavenumbers in units of cm^{-1}.

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quencies, Part 1 [1][2], Part 2 [2], Part 3 [3], Part 4, Part 5 [4], Part 6 [5], Part 7 [6], and Part 8 [7], and as the Consolidated Volumes I [8] and II [9]. These two volumes consist of the contents of the above eight parts, after revision in the light of new experimental data, and give a reliable set of fundamental frequencies for 435 basic molecules.

On preparing these tables of frequencies we chose the molecules for which almost all the required data were available from the infrared and Raman spectra, and we selected the most probable values of frequencies with a judgment of the accuracies of the values. In the course of preparing these tables we noticed that the further extension of the tables is limited, since for larger molecules the number of fundamental vibrational frequencies increases and it becomes more and more difficult to observe all of them in the infrared and Raman spectra. Accordingly we decided to adopt a different approach for preparing the further extension of such tables. The present article is the first of this series.

In the present approach we first tried to determine a set of force constants which explains all the frequencies of a group of small molecules for which the assignments had already been established. Then we calculated the frequencies of larger molecules and compared them with the observed when they were available. We chose the chain molecules consisting of the CH_3, CD_3, CH_2, CD_2, CHD, O, S, F, Cl, Br, and I groups. The result was successful as shown in a series of papers entitled "Vibration Spectra and Rotational Isomerism of Chain Molecules" [10–15]. The agreement between the calculated and the observed was less than 10 cm^{-1} with a few exceptions and shows that the frequency tables given by adopting this approach can be used as the extension of those of Parts 1–8.

In the present article we give the tables of force constants used and tables of the calculated and observed frequencies of basic paraffin, ether, sulfide, and thiaether molecules. We have suitable computer programs for calculating the frequencies of larger molecules, and we are prepared to perform the calculations and make the results available for any molecule upon request, provided that this is within the capacity of our programs.

2. Molecules Selected

The present part contains tables of fundamental vibrational frequences for 109 molecular forms of 38 chain molecules consisting of the CH_3, CH_2, O, S, and their deuterated atomic groups. The molecules are limited to those with four to six atomic groups except for the polymers $(CH_2)_n$, $(CD_2)_n$, $(OCH_2CH_2)_n$, $(OCD_2CD_2)_n$, $(SCH_2CH_2)_n$ and $(SCD_2CD_2)_n$. Rotational isomers included have been confirmed to exist except for the GG form of $CH_3CH_2OCH_2CH_3$. The following molecules are not included in the tables: molecules having the OO, SS, and XCH_2Y groups where X and Y are neither CH_3 nor CH_2.

A list of the molecules covered here is given at the beginning of the tables. The molecules are numbered starting with number 1 instead of continuing the designations of Part 8 of the tables, since the present part gives fundamental vibrational frequencies by adopting an approach different from that in the previous parts.

[2] Figures in brackets indicate literature references in section 7.

3. Calculation of Vibrational Frequencies

3.1. Computer Programs and Calculation

The programs used are based on a package of programs GCCC, BGLZ, LSMB, and LXZ prepared in our laboratory [16]. These programs were combined by Y. Alaki, Y. Omura, and H. Matsuura to NCTB which produces vibrational frequencies, vibrational modes and other data from the molecular structure and the force constants. It also can produce the force constants from the calculated and observed frequencies by the least-squares procedure.

In addition to NCTB we developed a program system named MVIB which is of the interacting type and is used for the remote TSS terminal. It was combined by H. Matsuura from NCTB2 revised from NCTB for this purpose and INPUT2 prepared by Shirley S. Hui which gives a set of input data for NCTB2 from the molecular formula and the indication of the conformation. The MVIB system uses the structure and force constant data stored in the computer files and calculates the frequencies and other data from the molecular formula with the conformation. The details of the normal coordinate treatment will be found in reference [17].

All of the calculations were made by the HITAC 8800/8700 Computing System at the Computer Center of the University of Tokyo.

3.2. Atomic Masses and Structural Parameters

The atomic masses and the structural parameters listed in table 1 were used in common in the calculations of vibrational frequencies of the molecules treated in this work. The structural parameters were taken from butane [18], ethyl methyl ether [19], and ethyl methyl sulfide [20].

The dihedral angles were assumed to be 180° (trans), 60° ($gauche^+$) and −60° ($gauche^-$) except for those of $(OCH_2CH_2)_n$, $(OCD_2CD_2)_n$, $(SCH_2CH_2)_n$ and $(SCD_2CD_2)_n$ for which the dihedral angles are indicated in their tables. The symbols t, g^+, and g^- are used for the trans, $gauche^+$ and $gauche^-$ conformations, respectively, in the notation of the force constants (section 3.4). The conformations of molecules, as given at the top of each of the tables of vibrational frequencies, are denoted generically by the symbols T, G, and G′. The details will be found in reference [10]. The gauche (G) and gauche′ (G′) forms of $CH_3OCHDCH_3$ and $CD_3OCHDCD_3$ correspond to the $gauche^+$ and $gauche^-$ conformations, respectively. The definition of the CHD group is given in table 2.

The definition of the dihedral angle will be found in references [21,22].

3.3. Local Symmetry Coordinates

The local symmetry coordinates defined in table 2 were adopted as basis coordinates in the calculations. For the coordinate systems of the CH_3 and CH_2 groups, the redundant

TABLE 1. Atomic masses and structural parameters used in the calculations

Property	Quantity
Atomic masses,[a] u	
Hydrogen (protium)	1.007825
Hydrogen (deuterium)	2.014102
Carbon	12.011
Oxygen	15.9994
Sulfur	32.06
Bond lengths, Å	
r(C-H)	1.100
r(C-C)	1.539
r(C-O)	1.410
r(C-S)	1.816
Bond angles, degree	
∡(C-C-C)	112.2
∡(C-C-O)	108.1
∡(C-C-S)	113.6
∡(C-O-C)	111.8
∡(C-S-C)	98.6
∡(C-C-H)	110.4
∡(O-C-H)	109.8
∡(S-C-H)	108.8
Dihedral angles, degree	
Trans conformation	180
Gauche⁺ conformation	60
Gauche⁻ conformation	−60

[a] The chemical masses (isotope abundance weighted) were used for the atoms other than hydrogen, since we do not consider the isotopic frequency shifts in these atoms in this article.

coordinates have been eliminated (see Appendix). The definition of the coordinates is based on the conventions recommended by IUPAC [22]. It should be noted that the signs of some of the coordinates depend on the direction of taking atomic groups. The signs of the coordinates are important since they are directly related to the signs of the off-diagonal force constants associated with these and other coordinates.

The local symmetry coordinates in a whole molecule are defined on the basis of the following conventions. (1) The signs of the coordinates for all of the non-terminal groups, e.g., CH_2, O, and S, in the molecule are positive, when one views the successive atomic groups constituting the molecule, in accordance with the molecular formula given in the tables of vibrational frequencies, from the left to the right. (2) The coordinates of the terminal groups, e.g., CH_3, can be defined uniquely, independent of the position of the groups (left-hand terminal or right-hand terminal) in the molecular formula, on the basis of the definition given in table 2. (3) The symmetry of the whole molecule is not taken into account in defining the basis coordinates for the normal coordinate calculations. The symmetry species of the vibrations are determined from the relative phase relations among the coordinates concerned.

3.4. Force Constants

The force constants are given in terms of the local symmetry coordinates [17]. Their values were determined by the least-squares procedure from experimental vibrational frequencies observed in infrared and Raman spectra. Detailed procedures of the least-squares calculations will be found in references [10,11,13,14]. The force constants which are characteristic of paraffins, ethers, sulfides and thiaethers are listed in tables 3–6. In these tables only the force constants with non-zero values are given and force constants not found in the tables have zero values. For the force constants determined by the least-squares procedure, the errors given in parentheses apply to the last significant figure(s). Other force constants were constrained to the values given in the tables or assumed to be equal to the corresponding force constants of similar groups.

Each of the force constants is given by the symbol consisting of four to seven characters which are grouped into the following three parts. The parts are divided by hyphens in the notation of the symbol. (1) The characters denoting the atomic groups to which the coordinates belong, (2) the character(s) denoting the coordinate(s), and (3) the character denoting the skeletal conformation. The symbols of the local symmetry coordinates and of the atomic groups are listed in table 2. The force constants are divided into two categories, the intragroup force constants and the intergroup force constants.

For the symbol of the intragroup force constant, the first three characters denote the atomic groups, the second implying the atomic group in question and the first and the third implying the two adjacent atomic groups, and the fourth character for the diagonal force constant (the fourth and fifth characters for the off-diagonal force constant) denote the coordinates in question. The coordinates are defined in accordance with the conventions given in section 3.3, so that

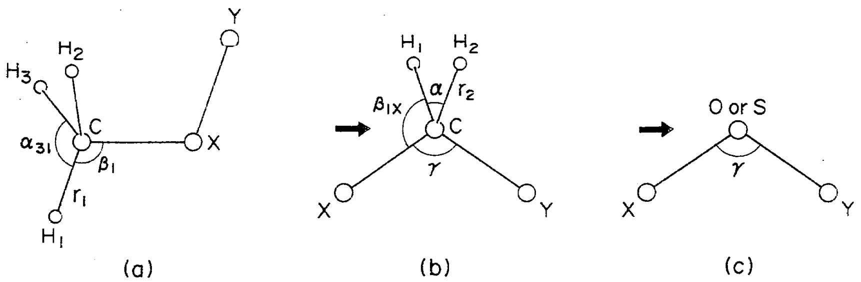

FIGURE 1. Parameters of atomic groups. (a) CH_3-(X), (b) (X)-CH_2-(Y), (c) (X)-O-(Y) or (X)-S-(Y). Arrows in (b) and (c) indicate the direction of viewing the atomic groups (see text).

TABLE 2. Definition and symbolism of local symmetry coordinates

Coordinate	Symbol	Definition
(a) CH_3-(X) group[a] (see figure 1a)		
CH_3 symmetrical stretching	1	$(\Delta r_1 + \Delta r_2 + \Delta r_3)/\sqrt{3}$
CH_3 symmetrical deformation	2	$a(\Delta\alpha_{23} + \Delta\alpha_{31} + \Delta\alpha_{12}) - b(\Delta\beta_1 + \Delta\beta_2 + \Delta\beta_3)$
CH_3 degenerate stretching	3	$(2\Delta r_1 - \Delta r_2 - \Delta r_3)/\sqrt{6}$
CH_3 degenerate deformation	4	$(2\Delta\alpha_{23} - \Delta\alpha_{31} - \Delta\alpha_{12})/\sqrt{6}$
CH_3 rocking	5	$(2\Delta\beta_1 - \Delta\beta_2 - \Delta\beta_3)/\sqrt{6}$
CH_3 degenerate stretching	6	$(\Delta r_2 - \Delta r_3)/\sqrt{2}$
CH_3 degenerate deformation	7	$(\Delta\alpha_{31} - \Delta\alpha_{12})/\sqrt{2}$
CH_3 rocking	8	$(\Delta\beta_2 - \Delta\beta_3)/\sqrt{2}$
(b) (X)-CH_2-(Y) group[a] (see figure 1b)		
CH_2 symmetrical stretching	1	$(\Delta r_1 + \Delta r_2)/\sqrt{2}$
CH_2 scissors	2	$c\Delta\alpha - d(\Delta\beta_{1X} + \Delta\beta_{2X}) - e(\Delta\beta_{1Y} + \Delta\beta_{2Y})$
CH_2 antisymmetrical stretching[b]	3	$(\Delta r_1 - \Delta r_2)/\sqrt{2}$
CH_2 rocking[b]	4	$(\Delta\beta_{1X} - \Delta\beta_{2X} + \Delta\beta_{1Y} - \Delta\beta_{2Y})/2$
CH_2 wagging[b]	5	$f(\Delta\beta_{1X} + \Delta\beta_{2X}) - g(\Delta\beta_{1Y} + \Delta\beta_{2Y})$
CH_2 twisting	6	$(\Delta\beta_{1X} - \Delta\beta_{2X} - \Delta\beta_{1Y} + \Delta\beta_{2Y})/2$
X-CH_2-Y deformation	D	$h\Delta\gamma - i\Delta\alpha - j(\Delta\beta_{1X} + \Delta\beta_{2X}) - k(\Delta\beta_{1Y} + \Delta\beta_{2Y})$
(c) (X)-O-(Y) or (X)-S-(Y) group[a] (see figure 1c)		
X-O-Y or X-S-Y bending	B	$\Delta\gamma$
(d) Other coordinates		
Skeletal stretching	S	
Torsion[c]	T	

$a = 0.414957$ and $b = 0.401428$ for X = C; $a = 0.410693$ and $b = 0.405789$ for X = O; $a = 0.403003$ and $b = 0.413427$ for X = S. $c = 0.906922$, $d = e = 0.210650$, $f = g = 1/2$, $h = 0.893737$, $i = 0.188991$ and $j = k = 0.203418$ for X = Y = C; $c = 0.891960$, $d = 0.227321$, $e = 0.224785$, $f = 0.497188$, $g = 0.502797$, $h = 0.911899$, $i = 0.185554$, $j = 0.184061$ and $k = 0.182007$ for X = C and Y = O; $c = 0.908651$, $d = 0.211232$, $e = 0.206296$, $f = 0.494055$, $g = 0.505875$, $h = 0.896457$, $i = 0.185032$, $j = 0.203691$ and $k = 0.198931$ for X = C and Y = S. For redundant coordinates, see Appendix.

[a] Symbols of atomic groups are 1 for CH_3, 1′ for CD_3, 2 for CH_2, 2′ for CD_2, 2″ for CHD, 3 for O, and 4 for S. The group CHD (2″) is defined in such a way that H_1 and H_2 in figure 1b are protium (H) and deuterium (D), respectively.

[b] The signs of the CH_2 antisymmetrical stretching, CH_2 rocking and CH_2 wagging coordinates of the (Y)-CH_2-(X) group (viewing the Y-CH_2-X group from the direction perpendicular to the HCH plane with the atom Y nearer to the observer) are opposite to those of the cooresponding coordinates of the (X)-CH_2-(Y) group (viewing the X-CH_2-Y group with the atom X nearer to the observer) [22]. The signs of the other coordinates are independent of the direction of viewing the atomic groups.

[c] The definition of the torsional coordinate will be found in references [21,22].

Table 3. Force constants of paraffins

Constant[a]	Value[b]	Constant[a]	Value[b]	Constant[a]	Value[b]
012-1	4.763	0122-86	-0.106(7)	1222-D5-t	=-2222-5D-t
012-2	0.585(3)	0122-S5	=-2222-5S	1222-DD-t	= 2222-DD-t
012-3	4.667	0122-SD	= 2222-DS	1222-44-g^+	= 2222-44-g^+
012-4	0.535(4)			*1222-45-g^+	= 2222-45-g^+
012-5	0.705(7)	1221-S	= 2222-S	1222-46-g^+	= 2222-46-g^+
012-6	= 012-3	1221-T	= 2222-T	*1222-4D-g^+	= 2222-4D-g^+
012-7	= 012-4	1221-5S	= 2222-5S	*1222-54-g^+	= 2222-45-g^+
012-8	= 012-5	1221-DS	= 2222-DS	1222-55-g^+	= 2222-55-g^+
012-45	0.024(5)	1221-22-t	= 2222-22-t	*1222-56-g^+	= 2222-56-g^+
012-78	= 012-45	1221-2D-t	= 2222-2D-t	1222-5D-g^+	= 2222-5D-g^+
		1221-44-t	= 2222-44-t	1222-64-g^+	=-2222-46-g^+
122-1	= 222-1	1221-46-t	= 2222-46-t	*1222-65-g^+	=-2222-56-g^+
122-2	= 222-2	1221-55-t	= 2222-55-t	1222-66-g^+	= 2222-66-g^+
122-3	= 222-3	1221-5D-t	= 2222-5D-t	*1222-6D-g^+	= 2222-6D-g^+
122-4	= 222-4	1221-66-t	= 2222-66-t	*1222-D4-g^+	=-2222-4D-g^+
122-5	= 222-5	1221-DD-t	= 2222-DD-t	1222-D5-g^+	=-2222-5D-g^+
122-6	= 222-6	1221-44-g^+	= 2222-44-g^+	*1222-D6-g^+	= 2222-6D-g^+
122-D	0.907(8)	*1221-45-g^+	= 2222-45-g^+	1222-DD-g^+	= 2222-DD-g^+
122-2D	= 222-2D	1221-46-g^+	= 2222-46-g^+		
122-SS	0.260(14)	*1221-4D-g^+	= 2222-4D-g^+	2222-S	4.453(7)
		1221-55-g^+	= 2222-55-g^+	2222-T	0.107
222-1	4.557	*1221-56-g^+	= 2222-56-g^+	2222-5S	-0.304(4)
222-2	0.589(2)	1221-5D-g^+	= 2222-5D-g^+	2222-DS	0.213(9)
222-3	4.519	1221-66-g^+	= 2222-66-g^+	2222-22-t	0.001(1)
222-4	0.766(5)	*1221-6D-g^+	= 2222-6D-g^+	2222-2D-t	0.042(7)
222-5	0.622(3)	1221-DD-g^+	= 2222-DD-g^+	2222-44-t	0.068(6)
222-6	0.639(4)			2222-46-t	0.063(7)
222-D	0.941(8)	1222-S	= 2222-S	2222-55-t	-0.042(2)
222-2D	0.047(12)	1222-T	= 2222-T	2222-5D-t	0.039(12)
222-SS	0.199(6)	1222-5S	= 2222-5S	2222-66-t	-0.070(2)
		1222-DS	= 2222-DS	2222-DD-t	0.105(8)
0122-S	4.450(5)	1222-S5	=-2222-5S	2222-44-g^+	-0.002(12)
0122-T	0.086	1222-SD	= 2222-DS	*2222-45-g^+	0.063(15)
0122-22	-0.005(7)	1222-22-t	= 2222-22-t	2222-46-g^+	-0.029(13)
0122-25	-0.034(10)	1222-2D-t	= 2222-2D-t	*2222-4D-g^+	-0.074(13)
0122-2D	-0.062(7)	1222-44-t	= 2222-44-t	2222-55-g^+	-0.014(6)
0122-2S	-0.436(10)	1222-46-t	= 2222-46-t	*2222-56-g^+	0.026(7)
0122-45	0.030(7)	1222-55-t	= 2222-55-t	2222-5D-g^+	-0.017(16)
0122-52	0.075(6)	1222-5D-t	= 2222-5D-t	2222-66-g^+	0.031(11)
0122-55	-0.053(7)	1222-64-t	=-2222-46-t	*2222-6D-g^+	0.079(20)
0122-5D	0.108(11)	1222-66-t	= 2222-66-t	2222-DD-g^+	0.048(23)
0122-84	-0.092(6)	1222-D2-t	= 2222-2D-t		

[a] The values of the g^- interaction constants are the same as those of the corresponding g^+ interaction constants, unless they are marked with *. For those marked with *, the absolute values of the g^+ and g^- interaction constants are the same but their signs are opposite to each other.

[b] Units are aJ $Å^{-2}$ = mdyn $Å^{-1}$ for the stretching and stretching–stretching constants, aJ $Å^{-1}$ = mdyn for the stretching-bending constants, and aJ = mdyn Å for the bending, bending-bending and torsional constants. Errors in the force constants, given in parentheses, apply to the last significant figure(s).

Table 4. Force constants of ethers

Constant[a]	Value[b]	Constant[a]	Value[b]	Constant[a]	Value[b]
012-2[c]	0.538(6)	0123-2D	0.104(16)	*1223-D6-g^+	= 2222-6D-g^+
012-7[c]	0.522(5)	0123-2S	-0.197(19)	1223-DD-g^+	= 2223-DD-g^+
		0123-45	0.019(11)		
013-1	4.575	0123-52	0.016(16)	1231-S	= 2232-S
013-2	0.679(13)	0123-55	-0.055(9)	1231-T	= 2232-T
013-3	4.746	0123-5D	0.099(14)	1231-2S	= 2232-2S
013-4	0.550(10)	0123-84	-0.130(41)	1231-5S	= 2232-5S
013-5	0.875(16)	0123-86	0.008(29)	1231-DS	= 2232-DS
013-6	= 013-3	0123-S2	= 2223-S2	1231-SB	= 2232-SB
013-7	0.539(9)	0123-S5	= 2223-S5	1231-2B-t	= 2232-2B-t
013-8	= 013-5	0123-SD	= 2223-SD	1231-5B-t	= 2232-5B-t
013-45	-0.022(12)			1231-DB-t	= 2232-DB-t
013-78	= 013-45	0132-S	5.145(16)	*1231-4B-g^+	= 2232-4B-g^+
		0132-T	0.066(3)	1231-5B-g^+	= 2232-5B-g^+
123-1	= 223-1	0132-2B	-0.072(19)	*1231-6B-g^+	= 2232-6B-g^+
123-2	= 223-2	0132-2S	-0.563(22)	1231-DB-g^+	= 2232-DB-g^+
123-3	= 223-3	0132-5B	0.012(25)		
123-4	= 223-4	0132-SB	= 2232-SB	1232-S	= 2232-S
123-5	= 223-5			1232-T	= 2232-T
123-6	= 223-6	1223-S	= 2223-S	1232-2S	= 2232-2S
123-D	1.120(25)	1223-T	= 2223-T	1232-5S	= 2232-5S
123-25	= 223-25	1223-5S	= 2222-5S	1232-DS	= 2232-DS
123-2D	= 223-2D	1223-DS	= 2222-DS	1232-SB	= 2232-SB
123-46	= 223-46	1223-S2	= 2223-S2	1232-2B-t	= 2232-2B-t
123-5D	= 223-5D	1223-S5	= 2223-S5	1232-5B-t	= 2232-5B-t
123-SS	0.371(28)	1223-SD	= 2223-SD	1232-DB-t	= 2232-DB-t
		1223-44-t	= 2223-44-t	*1232-4B-g^+	= 2232-4B-g^+
132-B	1.180(21)	1223-46-t	= 2222-46-t	1232-5B-g^+	= 2232-5B-g^+
132-SS	0.193(17)	1223-55-t	= 2223-55-t	*1232-6B-g^+	= 2232-6B-g^+
		1223-5D-t	= 2223-5D-t	1232-DB-g^+	= 2232-DB-g^+
223-1	4.580	1223-64-t	=-2222-46-t		
223-2	0.590(4)	1223-66-t	= 2223-66-t	2223-S	4.328(38)
223-3	4.672	1223-D2-t	= 2222-2D-t	2223-T	0.204(22)
223-4	0.820(31)	1223-D5-t	=-2222-5D-t	2223-5S	= 2222-5S
223-5	0.764(11)	1223-DD-t	= 2223-DD-t	2223-DS	= 2222-DS
223-6	0.699(16)	1223-2D-g^+	= 2223-2D-g^+	2223-S2	-0.102(17)
223-D	1.153(26)	1223-44-g^+	= 2223-44-g^+	2223-S5	0.279(20)
223-25	0.014(10)	*1223-45-g^+	= 2222-45-g^+	2223-SD	0.117(13)
223-2D	0.076(21)	1223-46-g^+	= 2222-46-g^+	2223-44-t	0.080(36)
223-46	-0.118(25)	*1223-4D-g^+	= 2223-4D-g^+	2223-46-t	= 2222-46-t
223-5D	0.128(17)	*1223-54-g^+	= 2222-45-g^+	2223-55-t	-0.044(12)
223-SS	0.314(28)	1223-55-g^+	= 2223-55-g^+	2223-5D-t	-0.003(18)
		*1223-56-g^+	= 2222-56-g^+	2223-64-t	=-2222-46-t
232-B	1.217(11)	1223-5D-g^+	= 2223-5D-g^+	2223-66-t	-0.038(13)
232-SS	0.248(21)	1223-64-g^+	=-2222-46-g^+	2223-D2-t	= 2222-2D-t
		*1223-65-g^+	=-2222-56-g^+	2223-D5-t	=-2222-5D-t
0123-S	4.510(35)	1223-66-g^+	= 2223-66-g^+	2223-DD-t	0.111(18)
0123-T	0.096(11)	*1223-6D-g^+	= 2223-6D-g^+	2223-2D-g^+	-0.046(20)
0123-22	-0.007(9)	*1223-D4-g^+	=-2222-4D-g^+	2223-44-g^+	-0.031(19)
0123-25	-0.013(7)	1223-D5-g^+	=-2222-5D-g^+	*2223-45-g^+	= 2222-45-g^+

Table 4. Force constants of ethers—Continued

Constant[c]	Value[b]	Constant[c]	Value[b]	Constant[c]	Value[b]
2223-46-g$^+$	= 2222-46-g$^+$	2231-5B-t	= 2232-5B-t	3223-T	0.123(20)
*2223-4D-g$^+$	-0.016(18)	2231-DB-t	= 2232-DB-t	3223-2S	= 2223-S2
*2223-54-g$^+$	= 2222-45-g$^+$	*2231-4B-g$^+$	= 2232-4B-g$^-$	3223-5S	=-2223-S5
2223-55-g$^+$	-0.022	2231-5B-g$^+$	= 2232-5B-g$^+$	3223-DS	0.037(23)
*2223-56-g$^+$	= 2222-56-g$^+$	*2231-6B-g$^+$	= 2232-6B-g$^+$	3223-44-t	0.011(29)
2223-5D-g$^+$	0.010(19)	2231-DB-g$^+$	= 2232-DB-g$^+$	3223-46-t	= 2222-46-t
2223-64-g$^+$	=-2222-46-g$^+$			3223-55-t	-0.041(33)
*2223-65-g$^+$	=-2222-56-g$^+$	2232-S	5.037(22)	3223-5D-t	= 2223-5D-t
2223-66-g$^+$	0.004(13)	2232-T	0.098(21)	3223-66-t	-0.054(36)
*2223-6D-g$^+$	0.072(18)	2232-2S	-0.176(24)	3223-DD-t	0.274(42)
*2223-D4-g$^+$	=-2222-4D-g$^+$	2232-5S	-0.588(22)	3223-2D-g$^+$	= 2223-2D-g$^+$
2223-D5-g$^+$	=-2222-5D-g$^+$	2232-DS	0.386(18)	3223-44-g$^+$	0.023(38)
*2223-D6-g$^+$	= 2222-6D-g$^+$	2232-SB	0.363(16)	*3223-45-g$^+$	= 2222-45-g$^+$
2223-DD-g$^+$	-0.010(21)	2232-2B-t	-0.030(22)	3223-46-g$^+$	= 2222-46-g$^+$
		2232-5B-t	-0.040(26)	*3223-4D-g$^+$	= 2223-4D-g$^+$
2231-S	= 2232-S	2232-DB-t	0.089(18)	3223-55-g$^+$	-0.031(9)
2231-T	= 2232-T	*2232-4B-g$^+$	-0.047(15)	*3223-56-g$^+$	= 2222-56-g$^+$
2231-2S	= 2232-2S	2232-5B-g$^+$	0.060(22)	3223-5D-g$^+$	= 2223-5D-g$^+$
2231-5S	= 2232-5S	*2232-6B-g$^+$	0.070(20)	3223-66-g$^+$	0.042(14)
2231-DS	= 2232-DS	2232-DB-g$^+$	0.185(25)	*3223-6D-g$^+$	= 2223-6D-g$^+$
2231-SB	= 2232-SB			3223-DD-g$^+$	0.166(29)
2231-2B-t	= 2232-2B-t	3223-S	= 2223-S	3223-DD-g^{+}[d]	-0.010(29)

[a] The values of the g$^-$ interaction constants are the same as those of the corresponding g$^+$ interaction constants, unless they are marked with *. For those marked with *, the absolute values of the g$^+$ and g$^-$ interaction constants are the same but their signs are opposite to each other.

[b] Units are aJ $\mathrm{Å}^{-2}$ = mdyn $\mathrm{Å}^{-1}$ for the stretching and stretching-stretching constants, aJ $\mathrm{Å}^{-1}$ = mdyn for the stretching-bending constants, and aJ = mdyn Å for the bending, bending-bending and torsional constants. Errors in the force constants, given in parentheses, apply to the last significant figure(s).

[c] Applicable only to the methyl group of the CH_3CH_2O part.

[d] Applicable only to $(OCH_2CH_2)_n$ and $(OCD_2CD_2)_n$.

Table 5. Force constants of sulfides

Constant[a]	Value[b]	Constant[a]	Value[b]	Constant[a]	Value[b]
014–1	4.715	0124–52	0.016(23)	1241–5S	= 2242–5S
014–2	0.559(8)	0124–55	−0.058(15)	1241–DS	= 2242–DS
014–3	4.637	0124–5D	0.067(35)	1241–SB	= 2242–SB
014–4	0.537(3)	0124–84	−0.064(16)	1241–2B–t	= 2242–2B–t
014–5	0.628(3)	0124–86	−0.117(15)	1241–5B–t	= 2242–5B–t
014–6	= 014–3	0124–S5	=−2222–5S	1241–DB–t	= 2242–DB–t
014–7	0.530(3)	0124–SD	= 2224–SD	*1241–4B–g$^+$	= 2242–4B–g$^+$
014–8	= 014–5			1241–5B–g$^+$	= 2242–5B–g$^+$
014–45	−0.020(5)	0142–S	3.104(36)	*1241–6B–g$^+$	= 2242–6B–g$^+$
014–78	= 014–45	0142–T	0.045	1241–DB–g$^+$	= 2242–DB–g$^+$
		0142–2B	0.194(26)		
124–1	= 224–1	0142–2S	−0.340(35)	1242–S	= 2242–S
124–2	= 224–2	0142–5B	0.003(13)	1242–T	= 2242–T
124–3	= 224–3	0142–SB	= 2242–SB	1242–5S	= 2242–5S
124–4	= 224–4			1242–DS	= 2242–DS
124–5	= 224–5	1224–S	= 2224–S	1242–SB	= 2242–SB
124–6	= 224–6	1224–T	= 2224–T	1242–2B–t	= 2242–2B–t
124–D	0.857(37)	1224–5S	= 2222–5S	1242–5B–t	= 2242–5B–t
124–25	= 224–25	1224–DS	= 2222–DS	1242–DB–t	= 2242–DB–t
124–2D	= 224–2D	1224–S5	=−2222–5S	*1242–4B–g$^+$	= 2242–4B–g$^+$
124–46	= 224–46	1224–SD	= 2224–SD	1242–5B–g$^+$	= 2242–5B–g$^+$
124–5D	= 224–5D	1224–2D–t	= 2224–2D–t	*1242–6B–g$^+$	= 2242–6B–g$^+$
124–SS	= 224–SS	1224–44–t	= 2224–44–t	1242–DB–g$^+$	= 2242–DB–g$^+$
		1224–46–t	= 2222–46–t		
142–B	1.358(33)	1224–55–t	= 2224–55–t	2224–S	4.424(26)
142–SS	= 242–SS	1224–5D–t	= 2224–5D–t	2224–T	0.113
		1224–64–t	=−2222–46–t	2224–5S	= 2222–5S
224–1	4.689	1224–66–t	= 2224–66–t	2224–DS	= 2222–DS
224–2	0.551(5)	1224–D2–t	= 2222–2D–t	2224–S5	=−2222–5S
224–3	4.637	1224–D5–t	=−2222–5D–t	2224–SD	0.035(36)
224–4	0.804(15)	1224–DD–t	= 2224–DD–t	2224–2D–t	−0.050(32)
224–5	0.607(11)	1224–44–g$^+$	= 2224–44–g$^+$	2224–44–t	0.058(17)
224–6	0.626(4)	*1224–45–g$^+$	= 2222–45–g$^+$	2224–46–t	= 2222–46–t
224–D	0.846(41)	1224–46–g$^+$	= 2222–46–g$^+$	2224–55–t	−0.047(12)
224–25	0.054(10)	*1224–4D–g$^+$	= 2224–4D–g$^+$	2224–5D–t	−0.034(30)
224–2D	0.161(35)	*1224–54–g$^+$	= 2222–45–g$^+$	2224–64–t	=−2222–46–t
224–46	−0.030(28)	1224–55–g$^+$	= 2224–55–g$^+$	2224–66–t	−0.074(15)
224–5D	0.113(30)	*1224–56–g$^+$	= 2222–56–g$^+$	2224–D2–t	= 2222–2D–t
224–SS	0.473(26)	1224–5D–g$^+$	= 2224–5D–g$^+$	2224–D5–t	=−2222–5D–t
		1224–64–g$^+$	=−2222–46–g$^+$	2224–DD–t	0.076(37)
242–B	1.481(22)	*1224–65–g$^+$	=−2222–56–g$^+$	2224–44–g$^+$	0.011(53)
242–SS	−0.066(33)	1224–66–g$^+$	= 2224–66–g$^+$	*2224–45–g$^+$	= 2222–45–g$^+$
		*1224–6D–g$^+$	= 2224–6D–g$^+$	2224–46–g$^+$	= 2222–46–g$^+$
0124–S	= 2224–S	*1224–D4–g$^+$	=−2222–4D–g$^+$	*2224–4D–g$^+$	−0.026(34)
0124–T	0.110(7)	1224–D5–g$^+$	=−2222–5D–g$^+$	*2224–54–g$^+$	= 2222–45–g$^+$
0124–22	−0.022(7)	*1224–D6–g$^+$	= 2222–6D–g$^+$	2224–55–g$^+$	0.070(20)
0124–25	−0.041(18)	1224–DD–g$^+$	= 2224–DD–g$^+$	*2224–56–g$^+$	= 2222–56–g$^+$
0124–2D	−0.040(23)			2224–5D–g$^+$	−0.036(57)
0124–2S	−0.345(28)	1241–S	= 2241–S	2224–64–g$^+$	=−2222–46–g$^+$
0124–45	0.025(23)	1241–T	= 2242–T	*2224–65–g$^+$	=−2222–56–g$^+$

Table 5. Force constants of sulfides—Continued

Constant[a]	Value[b]	Constant[a]	Value[b]	Constant[a]	Value[b]
2224-66-g$^+$	0.063(19)	2241-DB-g$^+$	= 2242-DB-g$^+$	4224-DS	-0.003(36)
*2224-6D-g$^+$	0.162(37)			4224-2D-t	= 2224-2D-t
*2224-D4-g$^+$	=-2222-4D-g$^+$	2242-S	2.959(57)	4224-44-t	0.085(28)
2224-D5-g$^+$	=-2222-5D-g$^+$	2242-T	0.045	4224-46-t	= 2222-46-t
*2224-D6-g$^+$	= 2222-6D-g$^+$	2242-5S	-0.217(44)	4224-55-t	-0.050(5)
2224-DD-g$^+$	-0.061(28)	2242-DS	0.226(30)	4224-5D-t	= 2224-5D-t
		2242-SB	0.058(27)	4224-66-t	-0.081(15)
2241-S	3.012(58)	2242-2B-t	-0.169(30)	4224-DD-t	0.031(41)
2241-T	= 2242-T	2242-5B-t	-0.091(27)	4224-44-g$^+$	-0.017(40)
2241-5S	= 2242-5S	2242-DB-t	0.149(41)	*4224-45-g$^+$	= 2222-45-g$^+$
2241-DS	= 2242-DS	*2242-4B-g$^+$	0.415(40)	4224-46-g$^+$	= 2222-46-g$^+$
2241-SB	= 2242-SB	2242-5B-g$^+$	-0.035(34)	*4224-4D-g$^+$	= 2224-4D-g$^+$
2241-2B-t	= 2242-2B-t	*2242-6B-g$^+$	0.070(31)	4224-55-g$^+$	0.041(15)
2241-5B-t	= 2242-5B-t	2242-DB-g$^+$	0.049(42)	*4224-56-g$^+$	= 2222-56-g$^+$
2241-DB-t	= 2242-DB-t			4224-5D-g$^+$	= 2224-5D-g$^+$
*2241-4B-g$^+$	= 2242-4B-g$^+$	4224-S	= 2224-S	4224-66-g$^+$	= 2224-66-g$^+$
2241-5B-g$^+$	= 2242-5B-g$^+$	4224-T	0.195(45)	*4224-6D-g$^+$	= 2224-6D-g$^+$
*2241-6B-g$^+$	= 2242-6B-g$^+$	4224-5S	= 2222-5S	4224-DD-g$^+$	-0.180(34)

[a] The values of the g$^-$ interaction constants are the same as those of the corresponding g$^+$ interaction constants, unless they are marked with *. For those marked with *, the absolute values of the g$^+$ and g$^-$ interaction constants are the same but their signs are opposite to each other.

[b] Units are aJ Å^{-2} = mdyn Å^{-1} for the stretching and stretching-stretching constants, aJ Å^{-1} = mdyn for the stretching-bending constants, and aJ = mdyn Å for the bending, bending-bending and torsional constants. Errors in the force constants, given in parentheses, apply to the last significant figure(s).

Table 6. Force constants of thiaethers

Constant[a]	Value[b]	Constant[a]	Value[b]	Constant[a]	Value[b]
3224-S	4.499(13)	3224-5D-t	= 2224-5D-t	*3224-56-g$^+$	= 2222-56-g$^+$
3224-T	0.123	3224-64-t	=-2222-46-t	3224-5D-g$^+$	= 2224-5D-g$^+$
3224-2S	= 2223-S2	3224-66-t	-0.067(7)	3224-64-g$^+$	=-2222-46-g$^+$
3224-5S	=-2223-S5	3224-D5-t	=-2223-5D-t	*3224-65-g$^+$	=-2222-56-g$^+$
3224-DS	= 2223-SD	3224-DD-t	0.214(14)	3224-66-g$^+$	0.067(27)
3224-S5	=-2222-5S	3224-44-g$^+$	-0.032(34)	*3224-6D-g$^+$	= 2224-6D-g$^+$
3224-SD	= 2224-SD	*3224-45-g$^+$	= 2222-45-g$^+$	3224-D2-g$^+$	= 2223-2D-g$^+$
3224-2D-t	= 2224-2D-t	3224-46-g$^+$	= 2222-46-g$^+$	*3224-D4-g$^+$	=-2223-4D-g$^+$
3224-44-t	-0.031(11)	*3224-4D-g$^+$	= 2224-4D-g$^+$	3224-D5-g$^+$	=-2223-5D-g$^+$
3224-46-t	= 2222-46-t	*3224-54-g$^+$	= 2222-45-g$^+$	*3224-D6-g$^+$	= 2223-6D-g$^+$
3224-55-t	-0.031(12)	3224-55-g$^+$	-0.060(76)	3224-DD-g$^+$	-0.001(39)

[a] The values of the g$^-$ interaction constants are the same as those of the corresponding g$^+$ interaction constants, unless they are marked with *. For those marked with *, the absolute values of the g$^+$ and g$^-$ interaction constants are the same but their signs are opposite to each other.

[b] Units are aJ Å^{-2} = mdyn Å^{-1} for the stretching and stretching-stretching constants, aJ Å^{-1} = mdyn for the stretching-bending constants, and aJ = mdyn Å for the bending, bending-bending and torsional constants. Errors in the force constants, given in parentheses, apply to the last significant figure(s).

their signs are positive when one views the successive atomic groups given by the first to third characters from the left to the right. If the atomic group in question is a terminal group, the nonexistent adjacent group is denoted by 0. Examples are given below.

012-2: the diagonal force constant for the CH_3 symmetrical deformation in the CH_3 group of the CH_3CH_2 part.

223-46: the off-diagonal force constant for the CH_2 rocking and the CH_2 twisting within the C^bH_2 group of the $C^aH_2C^bH_2O$ part.

242-SS: the off-diagonal force constant for the C^a-S stretching and S-C^b stretching of the $C^aH_2SC^bH_2$ part.

For the symbol of the intergroup force constant, the first four characters denote the atomic groups, the second and the third implying the two atomic groups in question and the first and the fourth implying their adjacent atomic groups, and the fifth character for the diagonal force constant (the fifth and sixth characters for the off-diagonal force constant) denote the coordinates in question. The coordinates given by the fifth and sixth characters belong, respectively, to the atomic groups given by the second and third characters. These coordinates are defined so that their signs are positive when one views the successive atomic groups given by the first to fourth characters from the left to the right. For the off-diagonal force constant associated with the skeletal stretching, this coordinate implies the stretching of the bond formed by the atomic groups denoted by the second and third characters. The seventh character, if any, denotes the conformation of the molecular skeleton given by the first to fourth characters. Examples of the symbols are given below.

2232-S: the diagonal force constant for the C^b-O stretching of the $C^aH_2C^bH_2OC^cH_2$ part.

0123-25: the off-diagonal force constant for the CH_3 symmetrical deformation and the CH_2 wagging of the CH_3CH_2O part.

2242-5S: the off-diagonal force constant for the C^bH_2 wagging and the C^b-S stretching of the $C^aH_2C^bH_2SC^cH_2$ part.

2223-46-g$^+$: the off-diagonal force constant for the C^bH_2 rocking and the C^cH_2 twisting of the $C^aH_2C^bH_2C^cH_2O$ part in the gauche$^+$ conformation.

It should be noted that the signs of some of the force constants are reversed if the force constants are defined by ordering the atomic groups in an opposite direction. Of the force constants listed in tables 3–6, only the following force constants have such sign reverse character: the off-diagonal intragroup or intergroup force constants for which one of the two coordinates is the CH_2 antisymmetrical stretching, the CH_2 rocking or the CH_2 wagging and the other coordinate is not any of these three coordinates. Thus, for example, 223-5D = -322-5D, 0122-S5 = -2210-5S, 2223-46-t = -3222-64-t, 2224-S5 = -4222-5S, etc.

Most of the intergroup force constants for the gauche$^-$ conformation are equivalent to the corresponding force constants for the gauche$^+$ conformation. For some of the force constants, however, the absolute values of the gauche$^+$ and gauche$^-$ constants are the same but their signs are opposite to each other. These force constants are marked with * in tables 3–6.

4. Description of Tables

4.1. Symmetry

The symmetry (point group) of each molecule is given by the Schoenflies notation. Detailed discussions of symmetry properties will be found in references [23,24].

4.2. Symmetry Number

The symmetry number, σ, is used in the calculation of thermodynamic quantities. It is the number of indistinguishable positions into which the molecule can be transformed by simple rigid rotations. A general discussion and pertinent formulas may be found in reference [24], page 508.

4.3. Symmetry Species

In the tables the normal modes are divided into the symmetry species of the point group to which the molecule belongs. The ordering of species in each point group is given in table I of reference [8], which is a summary of tables 12–30 of reference [24]. When a molecule has two or three planes of symmetry, the relationship between the vibrational modes and symmetry species cannot be defined uniquely. In such cases we generally follow the notation adopted in reference [24].

4.4. Observed Frequencies

The sources of the observed frequencies are given at the bottom of each of the tables. The infrared and Raman spectra of most of the molecules covered in this part were remeasured or newly measured in our laboratory. The abbreviations IR and R stand for infrared and Raman, respectively.

The observed frequencies used in the refinement of the force field are, as a general rule, those observed in the liquid state or in solution. For the cases where the bands of the liquid state or solution are not well resolved, the frequencies observed in the solid state, or in rarer cases, in the gaseous state are used. All the observed frequencies for polymer molecules are those in the solid state. Some of the observed frequencies reported in references are corrected for Fermi resonance.

The following abbreviations are used in the column for observed frequency to indicate the state of aggregation in which the frequency is observed. If no indication is given, the frequency is that observed in the liquid state or in solution.

(s) Observed in the solid state.

(g) Observed in the gaseous state.

4.5. Vibrational Assignment

Assignments of the vibrations are given by the calculated potential-energy distributions (P.E.D.) [25,26] in terms of the local symmetry coordinates. The values in parentheses are the potential energy distributions given by percent, and the signs denote relative phase relations among the coordinates

associated with the normal vibration. In the tables, the potential-energy distributions more than 10 percent are given with a maximum of four coordinates but, if the total of these distributions is less than 70 percent and if the number of the coordinates so far listed is smaller than four, additional distributions are also given until the total exceeds 70 percent.

The coordinates are given by the symbols which have the same format as that of the corresponding diagonal force constants. The arranging order of the atomic groups in the coordinate symbols is in accordance with the molecular formulas given in the tables. The symbols of the deuterated atomic groups are not distinguished from those of the corresponding undeuterated atomic groups in denoting them for the potential-energy distributions. Thus the symbol 1 is used for the CH_3 and CD_3 groups and the symbol 2 for the CH_2, CD_2, and CHD groups.

5. Appendix

In the coordinate systems of the CH_3 and CH_2 groups, the redundant coordinates have to be eliminated properly in defining the force constants in terms of the local symmetry coordinates.

The relation among the six angles ϕ_{12}, ϕ_{13}, ϕ_{14}, ϕ_{23}, ϕ_{24}, and ϕ_{34} about a carbon atom is expressed generally by

$$\begin{vmatrix} 1 & \cos\phi_{12} & \cos\phi_{13} & \cos\phi_{14} \\ \cos\phi_{12} & 1 & \cos\phi_{23} & \cos\phi_{24} \\ \cos\phi_{13} & \cos\phi_{23} & 1 & \cos\phi_{34} \\ \cos\phi_{14} & \cos\phi_{24} & \cos\phi_{34} & 1 \end{vmatrix} = 0. \quad \text{(A1)}$$

This relation gives the following redundancy function [27]

$$W = 2\Sigma a_{ij}(\Delta\phi_{ij}) + \Sigma b_{ij}(\Delta\phi_{ij})^2 + 2\Sigma c_{ij}(\Delta\phi_{ij})(\Delta\phi_{ik}) + 2\Sigma d_{ik}(\Delta\phi_{ij})(\Delta\phi_{kl}). \quad \text{(A2)}$$

Since the term linear in $\Delta\phi_{ij}$ corresponds to the redundant coordinate R,

$$R = 2\Sigma a_{ij}(\Delta\phi_{ij}), \quad \text{(A3)}$$

where $a_{ij} = 2(\cos\phi_{ij}^\circ - \cos\phi_{ij}^\circ \cos^2\phi_{kl}^\circ - \cos\phi_{ik}^\circ\cos\phi_{jk}^\circ - \cos\phi_{il}^\circ\cos\phi_{jl}^\circ + \cos\phi_{il}^\circ \cos\phi_{jk}^\circ \cos\phi_{kl}^\circ + \cos\phi_{ik}^\circ \cos\phi_{jl}^\circ\cos\phi_{kl}^\circ)$ $\sin\phi_{ij}^\circ$, and ϕ_{ij}° etc., are equilibrium values of ϕ_{ij} etc.

Since, for the (X)-CH_2-(Y) group (see figure 1b), $\phi_{12}^\circ = \alpha$, $\phi_{13}^\circ = \phi_{23}^\circ = \beta_X(=\beta_{1X}=\beta_{2X})$, $\phi_{14}^\circ = \phi_{24}^\circ = \beta_Y(=\beta_{1Y}=\beta_{2Y})$ and $\phi_{34}^\circ = \gamma$, equation (A3) is simplified as[3]

$$R = a\Delta\phi_{12} + b\Delta\phi_{34} + c(\Delta\phi_{13} + \Delta\phi_{23}) + d(\Delta\phi_{14}+\Delta\phi_{24}), \quad \text{(A4)}$$

where $a = \sin\alpha \sin^2\gamma$, $b = 2 \sin\gamma(2 \cos\beta_X\cos\beta_Y - \cos\alpha \cos\gamma - \cos\gamma)$, $c = 2 \sin\beta_X(\cos\beta_Y\cos\gamma - \cos\beta_X)$, and $d = 2 \sin\beta_Y(\cos\beta_X \cos\gamma - \cos\beta_Y)$. At the equilibrium position, equation (A1) gives the relation

$$\cos^2\beta_X + \cos^2\beta_Y - 2 \cos\beta_X \cos\beta_Y \cos\gamma = (1+\cos\alpha)(1-\cos^2\gamma)/2. \quad \text{(A5)}$$

[3] The coefficients a, b, and c appearing in equations (A4), (A7), and (A9) do not correspond to the coefficients a, b, and c in table 2.

By using equation (A5) and making the normalization, the redundant coordinate R is given by equation (A4) with the coefficients

$$\begin{aligned} a &= \sin\alpha \sin\gamma/N, \\ b &= 4AB/N, \\ c &= -2A \sin\beta_X/N, \\ d &= -2B \sin\beta_Y/N, \\ A &= \cos\beta_X\mathrm{cosec}\gamma - \cos\beta_Y\cot\gamma, \\ B &= \cos\beta_Y\mathrm{cosec}\gamma - \cos\beta_X\cot\gamma, \\ N &= (\sin^2\alpha \sin^2\gamma+16A^2B^2+8A^2 \sin^2\beta_X+8B^2 \sin^2\beta_Y)^{1/2}. \end{aligned} \quad \text{(A6)}$$

In the case of the (X)-CH_2-(X) group, for which $\phi_{12}^\circ = \alpha$, $\phi_{13}^\circ = \phi_{23}^\circ = \phi_{14}^\circ = \phi_{24}^\circ = \beta$ and $\phi_{34}^\circ = \gamma$, the redundant coordinate is given by

$$R = a\Delta\phi_{12} + b\Delta\phi_{34} + c(\Delta\phi_{13}+\Delta\phi_{23}+\Delta\phi_{14}+\Delta\phi_{24}). \quad \text{(A7)}$$

where

$$\begin{aligned} a &= \tan(\alpha/2)/N, \\ b &= \tan(\gamma/2)/N, \\ c &= -\tan\beta/2N, \\ N &= [\tan^2(\alpha/2) + \tan^2(\gamma/2) + \tan^2\beta]^{1/2}, \\ \cos^2\beta &= (1+\cos\alpha)(1 + \cos\gamma)/4. \end{aligned} \quad \text{(A8)}$$

In the case of the CH_3-(X) group (see figure 1a), for which $\phi_{12}^\circ = \phi_{13}^\circ = \phi_{23}^\circ = \alpha$ and $\phi_{14}^\circ = \phi_{24}^\circ = \phi_{34}^\circ = \beta$, the redundant coordinate is given by

$$R = a(\Delta\phi_{12}+\Delta\phi_{13}+\Delta\phi_{23}) + b(\Delta\phi_{14}+\Delta\phi_{24}+\Delta\phi_{34}), \quad \text{(A9)}$$

where

$$\begin{aligned} a &= \sin\alpha/N, \\ b &= -3 \cos\beta \sin\beta/N, \\ N &= (3 \sin^2\alpha+27 \cos^2\beta \sin^2\beta)^{1/2}, \\ \cos^2\beta &= (1+2 \cos\alpha)/3. \end{aligned} \quad \text{(A10)}$$

6. Acknowledgments

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7. References

[1] Shimanouchi, T., Tables of Molecular Vibrational Frequencies, Nat. Stand. Ref. Data Ser., Nat. Bur. Stand. (U.S.), 6, Part 1, 56 pages (March 1967).

[2] Shimanouchi, T., Tables of Molecular Vibrational Frequencies, Nat. Stand. Ref. Data Ser., Nat. Bur. Stand. (U.S.), 11, Part 2, 38 pages (October 1967).

[3] Shimanouchi, T., Tables of Molecular Vibrational Frequencies, Nat. Stand. Ref. Data Ser., Nat. Bur. Stand. (U.S.), 17, Part 3, 39 pages (March 1968).

[4] Shimanouchi, T., Tables of Molecular Vibrational Frequencies, Part 5, J. Phys. Chem. Ref. Data **1**, 189 (1972).

[5] Shimanouchi, T., Tables of Molecular Vibrational Frequencies, Part 6, J. Phys. Chem. Ref. Data **2**, 121 (1973).
[6] Shimanouchi, T., Tables of Molecular Vibrational Frequencies, Part 7, J. Phys. Chem. Ref. Data **2**, 225 (1973).
[7] Shimanouchi, T., Tables of Molecular Vibrational Frequencies, Part 8, J. Phys. Chem. Ref. Data **3**, 269 (1974).
[8] Shimanouchi, T., Tables of Molecular Vibrational Frequencies, Consolidated Volume I, Nat. Stand. Ref. Data Ser., Nat. Bur. Stand. (U.S.), 39, 164 pages (June 1972).
[9] Shimanouchi, T., Tables of Molecular Vibrational Frequencies, Consolidated Volume II, J. Phys. Chem. Ref. Data **6**, 993 (1977).
[10] Shimanouchi, T., Ogawa, Y., Ohta, M., Matsuura, H., and Harada, I., Bull. Chem. Soc. Jpn. **49**, 2999 (1976).
[11] Harada, I., Takeuchi, H., Sakakibara, M., Matsuura, H., and Shimanouchi, T., Bull. Chem. Soc. Jpn. **50** 102 (1977).
[12] Sakakibara, M., Matsuura, H., Harada, I., and Shimanouchi, T., Bull. Chem. Soc. Jpn. **50**, 111 (1977).
[13] Ohta, M., Ogawa, Y., Matsuura, H., Harada, I., and Shimanouchi, T., Bull. Chem. Soc. Jpn. **50**, 380 (1977).
[14] Ogawa, Y., Ohta, M., Sakakibara, M., Matsuura, H., Harada, I., and Shimanouchi, T., Bull. Chem. Soc. Jpn. **50**, 650 (1977).
[15] Matsuura, H., Kono, M., Iizuka, H., Ogawa, Y., Harada, I., and Shimanouchi, T., Bull. Chem. Soc. Jpn. **50**, 2272 (1977).
[16] Shimanouchi, T., Computer Programs for Normal Coordinate Treatment of Polyatomic Molecules (Department of Chemistry, Faculty of Science, University of Tokyo, 1968).
[17] Shimanouchi, T., The Molecular Force Field, Chapter 6 in Physical Chemistry, An Adv. Treatise, Volume IV. Molecular Properties, pp. 233–306, H. Eyring, D. Henderson and W. Jost, Ed. (Academic Press, New York, 1970).
[18] Kuchitsu, K., Bull. Chem. Soc. Jpn. **32**, 748 (1959).
[19] Hayashi, M., and Kuwada, K., J. Mol. Structure **28**, 147 (1975).
[20] Oyanagi, K., and Kuchitsu, K., 36th Annual Meeting of the Chemical Society of Japan (Osaka, 1977), 1M05.
[21] Miyazawa, T., and Fukushima, K., J. Mol. Spectrosc. **15**, 308 (1965).
[22] Information Bulletin, Appendices on Provisional Nomenclature, Symbols, Terminology, and Conventions Number 56, Definition and Symbolism of Molecular Force Constants, International Union of Pure and Applied Chemistry (December 1976).
[23] Wilson, E. B., Jr., Decius, J. C., and Cross, P. C., Molecular Vibrations (McGraw-Hill Book Co., New York, 1955).
[24] Herzberg, G., Infrared and Raman Spectra of Polyatomic Molecules (D. Van Nostrand, Inc. New York, 1945).
[25] Morino, Y., and Kuchitsu, K., J. Chem. Phys. **20**, 1809 (1952).
[26] Nakagawa, I., Nippon Kagaku Zasshi (J. Chem. Soc. Jpn., Pure Chem. Sect.) **74**, 243 (1953).
[27] Onishi, T., and Shimanouchi, T., Spectrochim. Acta **20**, 325 (1964).

8. List of Tables of Molecular Vibrational Frequencies

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No. 1
Molecule: 1221-T $CH_3CH_2CH_2CH_3$ ***(trans form)***
Symmetry C_{2h} **Symmetry number $\sigma = 2$**

Sym. species	Observed frequency cm^{-1}	Calculated frequency cm^{-1}	Assignment (P.E.D. %)			
a_g	1468	1469	210-4 (29+)	012-4 (29+)	221-2 (13+)	122-2 (13+)
	1441	1451	221-2 (34+)	122-2 (34+)	012-4 (13-)	210-4 (13-)
	1377(s)	1381	012-2 (51+)	210-2 (51+)		
	1360	1359	122-5 (42+)	221-5 (42-)	1221-S(18+)	
	1150	1151	012-5 (18+)	210-5 (18+)	1221-S(17-)	122-D (9+)
	1058	1052	0122-S(31+)	2210-S(31+)	1221-S(27-)	
	837	833	1221-S(45-)	210-5 (21-)	012-5 (21-)	
	430	429	221-D (33+)	122-D (33+)	0122-S(7+)	
a_u	1459(s)	1464	210-7 (41+)	012-7 (41+)		
	1258	1258	221-6 (29+)	122-6 (29+)	012-8 (8-)	210-8 (8-)
	948	952	012-8 (28+)	210-8 (28+)	122-6 (27+)	221-6 (27+)
	732	728	221-4 (43-)	122-4 (43+)		
		209	0122-T(46+)	2210-T(46+)		
		122	1221-T(90+)			
b_g	1455	1462	012-7 (41-)	210-7 (41+)		
	1303	1300	122-6 (40-)	221-6 (40+)		
	1181	1180	221-4 (21+)	122-4 (21+)	210-8 (17+)	012-8 (17-)
	805(s)	804	210-8 (27-)	012-8 (27+)	122-4 (25+)	221-4 (25+)
		244	2210-T(49+)	0122-T(49-)		
b_u		1487	122-2 (36-)	221-2 (36+)		
	1451(s)	1451	210-4 (35-)	012-4 (35+)	221-2 (11+)	122-2 (11-)
	1378	1378	210-2 (53+)	012-2 (53-)		
	1291	1295	221-5 (41+)	122-5 (41+)		
	1009(s)	1012	2210-S(50+)	0122-S(50-)		
	964	976	012-5 (33-)	210-5 (33+)	122-5 (14-)	221-5 (14-)
		265	122-D (57+)	221-D (57-)		

Calculated frequencies higher than 2000 cm^{-1}

2963 2962 2962 2962 2909 2900 2880 2880 2872 2865

References

[1] IR. R. G. Snyder and J. H. Schachtschneider, Spectrochim. Acta, **19**, 85 (1963).

[2] IR. R. G. Snyder, J. Chem. Phys., **47**, 1316 (1967).

[3] R. I. Harada, H. Takeuchi, M. Sakakibara, H. Matsuura, and T. Shimanouchi, Bull. Chem. Soc. Jpn., **50**, 102 (1977).

No. 2

Molecule: 1221-G $CH_3CH_2CH_2CH_3$ (gauche form)

Symmetry C_2 Symmetry number $\sigma = 2$

Sym. species	Observed frequency cm^{-1}	Calculated frequency cm^{-1}	Assignment (P.E.D. %)			
a		1484	122-2 (38+)	221-2 (38+)		
	1459*(s)	1463	210-7 (40+)	012-7 (40+)		
	1441*	1458	210-4 (36+)	012-4 (36+)		
	1377*(s)	1382	012-2 (51+)	210-2 (51+)		
	1338	1338	221-5 (33+)	122-5 (33-)	1221-S(18-)	
	1281	1275	122-6 (31+)	221-6 (31+)	221-5 (3+)	122-5 (3-)
	1168	1173	122-4 (14+)	221-4 (14-)	012-8 (10-)	210-8 (10-)
	1076	1083	1221-S(27+)	0122-S(20-)	2210-S(20-)	221-5 (7+)
	979	979	2210-S(18-)	0122-S(18-)	210-5 (15+)	012-5 (15+)
	829	829	1221-S(43-)	210-5 (14-)	012-5 (14-)	
	789	795	122-4 (24-)	221-4 (24+)	012-8 (18-)	210-8 (18-)
	323	321	122-D (32+)	221-D (32+)	0122-T(11+)	2210-T(11+)
		210	0122-T(35+)	2210-T(35+)	221-D (12-)	122-D (12-)
		121	1221-T(84+)			
b	1468*	1474	221-2 (25-)	122-2 (25+)	210-4 (16-)	012-4 (16+)
	1455*	1463	012-7 (39+)	210-7 (39-)		
	1451*(s)	1451	012-4 (25-)	210-4 (25+)	122-2 (20+)	221-2 (20-)
	1378	1379	210-2 (53-)	012-2 (53+)		
	1343	1348	122-5 (40+)	221-5 (40+)		
	1258	1259	221-6 (30+)	122-6 (30-)	012-8 (7+)	210-8 (7-)
	1132	1130	012-5 (15+)	210-5 (15-)	0122-S(9-)	2210-S(9+)
	964	963	012-5 (17-)	210-5 (17+)	210-8 (14+)	012-8 (14-)
	956	952	0122-S(35-)	2210-S(35+)	122-6 (7+)	
	748	750	221-4 (34+)	122-4 (34+)	210-8 (14-)	012-8 (14+)
		435	221-D (46+)	122-D (46-)		
		210	2210-T(46-)	0122-T(46+)		

Calculated frequencies higher than 2000 cm^{-1}

2963 2962 2962 2962 2907 2903 2880 2880 2870 2867

* Weight of the observed frequency is zero.

References

[1] IR. R. G. Snyder, J. Chem. Phys., **47**, 1316 (1967).

[2] R. I. Harada, H. Takeuchi, M. Sakakibara, H. Matsuura, and T. Shimanouchi, Bull. Chem. Soc. Jpn., **50**, 102 (1977).

No. 3
Molecule: 12221-TT $CH_3CH_2CH_2CH_2CH_3$ **(trans-trans form)**
Symmetry C_{2v} **Symmetry number** $\sigma = 2$

Sym. species	Observed frequency cm^{-1}	Calculated frequency cm^{-1}	Assignment (P.E.D. %)			
a_1	1477(s)	1486	222-2 (35+)	122-2 (19−)	221-2 (19−)	
	1458	1458	222-2 (42+)	210-4 (25+)	012-4 (25+)	
	1438	1446	221-2 (29+)	122-2 (29+)	222-2 (20+)	012-4 (10−)
	1379	1379	012-2 (52+)	210-2 (52+)		
	1328	1332	122-5 (43−)	221-5 (43+)		
	1146	1148	012-5 (15+)	210-5 (15+)	1222-S(11−)	2221-S(11−)
	1038	1042	0122-S(37−)	2210-S(37−)		
	868	868	210-5 (25−)	012-5 (25−)	2221-S(20−)	1222-S(20−)
	403	400	222-D (33+)	221-D (9+)	122-D (9+)	2210-S(7+)
	190	184	222-D (53−)	221-D (34+)	122-D (34+)	
a_2	1465	1463	012-7 (41+)	210-7 (41+)		
	1303	1304	222-6 (45+)	122-6 (18−)	221-6 (18−)	
	1238	1238	222-6 (24+)	221-6 (13+)	122-6 (13+)	012-8 (9−)
	986	981	222-6 (27+)	012-8 (20+)	210-8 (20+)	122-6 (20+)
	766	759	122-4 (37−)	221-4 (37+)	210-8 (15−)	012-8 (15−)
		229	2210-T(45+)	0122-T(45+)		
		122	2221-T(45+)	1222-T(45+)		
b_1	1473(s)	1478	122-2 (34−)	221-2 (34+)	012-4 (10−)	210-4 (10+)
	1458	1454	012-4 (32−)	210-4 (32+)	221-2 (13−)	122-2 (13+)
	1379	1380	210-2 (50+)	012-2 (50−)		
	1365	1367	222-5 (39−)	122-5 (23+)	221-5 (23+)	1222-S(13+)
	1263	1264	222-5 (53+)	221-5 (15+)	122-5 (15+)	
	1068	1068	2221-S(30+)	1222-S(30−)	122-5 (8+)	221-5 (8+)
	1027	1021	2210-S(30+)	0122-S(30−)	210-5 (14−)	012-5 (14+)
	920	927	0122-S(17+)	2210-S(17−)	012-5 (14+)	210-5 (14−)
	403	404	122-D (48−)	221-D (48+)		
b_2	1465	1463	210-7 (41−)	012-7 (41+)		
	1294	1288	221-6 (37+)	122-6 (37−)		
	1179	1177	222-4 (18+)	221-4 (16+)	122-4 (16+)	210-8 (13+)
	857(s)	857	222-4 (30+)	210-8 (25−)	012-8 (25+)	221-6 (13−)
	728	726	222-4 (40−)	221-4 (25+)	122-4 (25+)	
		233	0122-T(47−)	2210-T(47+)		
		104	1222-T(41+)	2221-T(41−)		

Calculated frequencies higher than 2000 cm^{-1}
2962 2962 2962 2962 2911 2904 2899 2880 2880 2874
2868 2864

References

[1] IR. R. G. Snyder and J. H. Schachtschneider, Spectrochim. Acta, **19**, 85 (1963).

[2] IR. R. G. Snyder, J. Chem. Phys., **47**, 1316 (1967).

[3] IR. A. Tomonaga and T. Shimanouchi, Bull. Chem. Soc. Jpn., **41**, 1446 (1968).

[4] R. I. Harada, H. Takeuchi, M. Sakakibara, H. Matsuura, and T. Shimanouchi, Bull. Chem. Soc. Jpn., **50**, 102 (1977).

No. 4
Molecule: 12221-TG $CH_3CH_2CH_2CH_2CH_3$ (trans-gauche form)
Symmetry C_1 Symmetry number $\sigma = 1$

Sym. species	Observed frequency cm^{-1}	Calculated frequency cm^{-1}	Assignment (P.E.D. %)			
a	1477*(s)	1488	222-2 (37+)	122-2 (24-)	221-2 (20+)	
	1473*(s)	1478	221-2 (43+)	122-2 (18+)	210-4 (18+)	
	1465*	1465	210-7 (44+)	222-2 (18+)	012-4 (8+)	210-8 (8+)
	1465*	1463	012-7 (81+)	012-8 (14+)		
	1458*	1461	210-7 (36+)	222-2 (20-)	210-4 (15+)	012-4 (13-)
	1450	1453	210-4 (31+)	012-4 (28+)	221-2 (16-)	122-2 (11-)
	1450	1451	122-2 (32+)	012-4 (20-)	222-2 (16+)	210-4 (12+)
	1379	1381	210-2 (83+)	012-2 (14-)		
	1379	1379	012-2 (89+)	210-2 (16+)		
	1365	1364	222-5 (41-)	122-5 (34+)	1222-S(15+)	
	1343	1344	221-5 (69+)	2221-S(12-)		
	1303	1301	122-5 (27+)	222-6 (16+)	222-5 (16+)	221-6 (14+)
	1300	1295	122-6 (40-)	222-6 (13+)	122-5 (12-)	222-5 (11-)
	1265	1263	221-6 (42-)	222-5 (14+)	210-8 (10+)	210-7 (7-)
	1238	1237	222-6 (34+)	122-6 (14+)	012-8 (13-)	122-4 (9+)
	1167	1167	222-4 (14-)	122-4 (11-)	221-4 (9+)	012-8 (9+)
	1140	1139	1222-S(16+)	012-5 (14-)	210-5 (9+)	222-D (6-)
	1075	1082	2221-S(30-)	2210-S(26+)	1222-S(11+)	221-5 (7-)
	1027	1028	0122-S(65-)	1222-S(12+)		
	1015	1014	012-5 (21+)	210-8 (14-)	222-5 (13+)	221-6 (12-)
	992	988	222-6 (23+)	012-8 (16+)	2210-S(16+)	122-6 (16+)
	909	908	210-5 (21+)	2210-S(19+)	1222-S(16-)	2221-S(13+)
	868	862	210-8 (18-)	222-4 (16-)	012-5 (11-)	012-8 (11-)
	841	846	222-4 (21+)	012-8 (18+)	2210-S(18-)	2221-S(10-)
	766	766	221-4 (43-)	210-8 (20+)	122-4 (17-)	
	733	732	122-4 (43+)	222-4 (27-)	221-4 (12-)	
	471	467	221-D (32+)	222-D (28-)	122-D (14-)	
	337	337	221-D (46+)	122-D (33+)		
	276	281	122-D (32+)	2210-T(31-)	222-D (29-)	
		228	0122-T(90-)			
		194	2210-T(60+)	222-D (25-)	122-D (10+)	
		112	2221-T(74+)			
		97	1222-T(83+)			

Calculated frequencies higher than 2000 cm^{-1}
2963 2962 2962 2962 2910 2905 2900 2880 2880 2873
2869 2865

* Weight of the observed frequency is zero.

References

[1] IR. R. G. Snyder, J. Chem. Phys., **47**, 1316 (1967).
[2] IR. A. Tomonaga and T. Shimanouchi, Bull. Chem. Soc. Jpn., **41**, 1446 (1968).
[3] R. I. Harada, H. Takeuchi, M. Sakakibara, H. Matsuura, and T. Shimanouchi, Bull. Chem. Soc. Jpn., **50**, 102 (1977).

No. 5
Molecule: 12221-GG $CH_3CH_2CH_2CH_2CH_3$ (gauche-gauche form)
Symmetry C_2 Symmetry number $\sigma = 2$

Sym. species	Observed frequency cm^{-1}	Calculated frequency cm^{-1}	Assignment (P.E.D. %)			
a	1477*(s)	1489	222-2 (40+)	122-2 (24+)	221-2 (24+)	
	1465*	1470	222-2 (32-)	210-4 (16+)	012-4 (16+)	122-2 (7+)
	1458*	1462	012-7 (36+)	210-7 (36+)		
	1450*	1451	012-4 (22+)	210-4 (22+)	222-2 (17+)	122-2 (15-)
	1379*	1379	210-2 (53+)	012-2 (53+)		
	1337	1341	221-5 (35+)	122-5 (35-)	222-6 (12-)	
		1279	122-6 (28+)	221-6 (28+)	222-6 (16+)	
	1223	1231	222-6 (42+)	221-6 (5-)	122-6 (5-)	210-8 (5+)
	1140*	1134	122-4 (12-)	221-4 (12+)	012-8 (9+)	210-8 (9+)
	1015*	1017	210-5 (22+)	012-5 (22+)	221-5 (13-)	122-5 (13+)
	986*	987	0122-S(33-)	2210-S(33-)	222-6 (17-)	
	841*	847	210-8 (15+)	012-8 (15+)	1222-S(14+)	2221-S(14+)
	766*	773	122-4 (18-)	221-4 (18+)	2221-S(16+)	1222-S(16+)
	471*	469	222-D (44+)	122-D (23-)	221-D (23-)	
	276*	266	221-D (21+)	122-D (21+)	222-D (20+)	0122-T(15+)
		191	2210-T(31-)	0122-T(31-)	222-D (23+)	
		72	1222-T(45+)	2221-T(45+)		
b	1473*(s)	1477	221-2 (31+)	122-2 (31-)	210-4 (12+)	012-4 (12-)
	1465*	1463	210-7 (41+)	012-7 (41-)		
	1450*	1455	210-4 (29+)	012-4 (29-)	221-2 (15-)	122-2 (15+)
	1379*	1382	012-2 (50-)	210-2 (50+)		
	1365*	1356	222-5 (42+)	122-5 (19+)	221-5 (19+)	
	1343*	1342	222-5 (25+)	122-5 (19-)	221-5 (19-)	1222-S(12-)
	1265*	1259	221-6 (24+)	122-6 (24-)	222-5 (8-)	012-8 (7+)
	1167*	1159	222-4 (14-)	2221-S(13-)	1222-S(13+)	012-5 (13-)
	1084	1092	0122-S(18-)	2210-S(18+)	1222-S(13+)	2221-S(13-)
	1015*	1006	222-5 (17-)	210-8 (15+)	012-8 (15-)	122-6 (13-)
	900	896	012-5 (21+)	210-5 (21-)	1222-S(15+)	2221-S(15-)
	858*	852	222-4 (41-)	2210-S(10+)	0122-S(10-)	012-8 (9+)
	733*	733	221-4 (31+)	122-4 (31+)	222-4 (16+)	210-8 (10-)
	384	385	122-D (38+)	221-D (38-)		
		230	0122-T(43-)	2210-T(43+)		
		135	2221-T(37-)	1222-T(37+)	222-4 (10-)	

Calculated frequencies higher than 2000 cm^{-1}

2962 2962 2962 2962 2908 2906 2902 2880 2880 2871
2868 2867

* Weight of the observed frequency is zero.

References

[1] IR. R. G. Snyder. J. Chem. Phys., **47**, 1316 (1967).
[2] IR. A. Tomonaga and T. Shimanouchi, Bull. Chem. Soc. Jpn., **41**, 1446 (1968).
[3] R. I. Harada, H. Takeuchi, M. Sakakibara, H. Matsuura, and T. Shimanouchi, Bull. Chem. Soc. Jpn., **50**, 102 (1977).

No. 6
Molecule: 1'2'2'2'1'-TT $CD_3CD_2CD_2CD_2CD_3$ (trans-trans form)
Symmetry C_{2v} Symmetry number $\sigma = 2$

Sym. species	Observed frequency cm^{-1}	Calculated frequency cm^{-1}	Assignment (P.E.D. %)			
a_1	1184	1178	2210-S(26+)	0122-S(26+)	221-5 (18+)	122-5 (18-)
	1135	1129	222-2 (29+)	1222-S(13+)	2221-S(13+)	222-D (9-)
	1090	1075	222-2 (29-)	221-2 (21+)	122-2 (21+)	122-5 (10+)
	1055(s)	1053	210-2 (34+)	012-2 (34+)	221-2 (10-)	122-2 (10-)
	1049(s)	1042	210-4 (36-)	012-4 (36-)		
	968	964	222-2 (15+)	221-2 (8+)	122-2 (8+)	012-2 (6+)
	863	862	122-5 (12+)	221-5 (12-)	2210-S(12+)	0122-S(12+)
	692	688	210-5 (31-)	012-5 (31-)	2221-S(11-)	1222-S(11-)
	358	358	222-D (33+)	122-D (9+)	221-D (9+)	2210-S(6+)
	157	159	222-D (51-)	122-D (34+)	221-D (34+)	
a_2	1049(s)	1045	012-7 (41+)	210-7 (41+)		
	968	976	222-6 (23+)	012-8 (11-)	210-8 (11-)	221-4 (11-)
	934	936	222-6 (32-)	221-6 (22+)	122-6 (22+)	
		714	222-6 (39-)	122-6 (25-)	221-6 (25-)	012-8 (13-)
	550(s)	558	122-4 (34-)	221-4 (34+)	210-8 (18-)	012-8 (18-)
		170	2210-T(42+)	0122-T(42+)		
		96	1222-T(42+)	2221-T(42+)		
b_1	1238	1235	1222-S(38+)	2221-S(38-)	222-5 (25-)	122-5 (13+)
	1119(s)	1118	122-2 (27+)	221-2 (27-)	2210-S(17-)	0122-S(17+)
	1057	1056	012-2 (38-)	210-2 (38+)	122-2 (10+)	221-2 (10-)
	1049(s)	1045	012-4 (43+)	210-4 (43-)		
	1008	1008	222-5 (45+)	221-5 (12+)	122-5 (12+)	012-5 (10-)
	881	883	0122-S(20-)	2210-S(20+)	221-2 (6-)	122-2 (6+)
	842	835	221-5 (15-)	122-5 (15-)	222-5 (13+)	2221-S(11-)
	730	728	012-5 (24-)	210-5 (24+)	222-5 (14-)	122-5 (10-)
		343	221-D (45+)	122-D (45-)		
b_2	1049(s)	1046	210-7 (40+)	012-7 (40-)		
	984	986	222-4 (25+)	122-4 (16+)	221-4 (16+)	012-7 (5+)
	967(s)	962	122-6 (28-)	221-6 (28+)	210-8 (10-)	012-8 (10+)
	638	635	222-4 (26-)	012-8 (26-)	210-8 (26+)	221-6 (19+)
	528	526	222-4 (39+)	221-4 (25-)	122-4 (25-)	
		169	0122-T(47-)	2210-T(47+)		
		88	2221-T(41-)	1222-T(41+)		

Calculated frequencies higher than 2000 cm^{-1}

2213 2213 2212 2212 2178 2161 2148 2130 2112 2098
2076 2075

Reference

[1] IR.R. I. Harada, H. Takeuchi, M. Sakakibara, H. Matsuura, and T. Shimanouchi, Bull. Chem. Soc. Jpn., **50**, 102 (1977).

No. 7
Molecule: 1'2'2'2'1'-TG $CD_3CD_2CD_2CD_2CD_3$ **(trans-gauche form)**
Symmetry C_1 **Symmetry number** $\sigma = 1$

Sym. species	Observed frequency cm^{-1}	Calculated frequency cm^{-1}	Assignment (P.E.D. %)			
a	1230	1229	1222-S(42+)	2221-S(33-)	222-5 (23-)	122-5 (20+)
	1184	1184	221-5 (33-)	2210-S(32-)	2221-S(21+)	1222-S(10+)
	1142	1143	221-2 (28+)	2210-S(19+)	222-2 (13+)	0122-S(11-)
	1125	1127	122-2 (30+)	0122-S(29+)	012-2 (14+)	
	1074	1068	222-2 (32-)	122-2 (23+)	122-5 (11+)	221-5 (4-)
	1057	1055	210-2 (72+)	221-2 (19-)		
	1057	1053	012-2 (66-)	122-2 (15+)		
	1049*(s)	1050	210-7 (29+)	222-5 (12+)	012-4 (12-)	221-2 (10-)
	1049*(s)	1046	012-7 (75+)	012-8 (12+)		
	1049*(s)	1043	210-7 (38+)	012-4 (37+)		
	1036	1039	210-4 (77-)			
	1036	1031	012-4 (33+)	222-5 (16+)	122-5 (13+)	210-7 (12-)
	984	982	122-4 (22+)	222-4 (17+)	012-8 (10-)	012-7 (9+)
	968	972	210-8 (13-)	221-4 (11-)	222-6 (9-)	012-8 (7+)
	953	958	122-6 (32-)	221-6 (19-)	210-8 (8+)	012-8 (8+)
	942	947	221-6 (12-)	122-2 (12-)	012-5 (9-)	222-2 (9-)
	934	938	222-6 (26+)	122-6 (14-)	210-5 (11+)	221-2 (7+)
	873	876	2210-S(16-)	221-5 (15+)	0122-S(9-)	2221-S(8+)
	853	853	122-5 (23-)	0122-S(19-)	1222-S(10+)	222-5 (9+)
	764	767	222-5 (20+)	221-5 (19-)	221-6 (15-)	210-5 (9+)
	753	754	222-6 (25-)	2210-S(20-)	221-6 (11+)	2221-S(8-)
	723	723	210-5 (24+)	012-5 (14-)	222-6 (12-)	221-5 (10-)
	692	688	012-5 (35-)	1222-S(17-)	221-6 (10-)	2221-S(10-)
	641	641	222-4 (32+)	012-8 (32+)	122-6 (27+)	
	575	577	221-4 (45+)	210-8 (38-)		
	542	540	122-4 (54-)	222-4 (20+)	012-8 (17-)	
	397	397	222-D (26-)	221-D (22+)	122-D (16-)	221-4 (9+)
	287	287	221-D (47+)	122-D (33+)		
	233	228	222-D (35+)	122-D (31-)	2210-T(22+)	
		167	0122-T(90+)			
		144	2210-T(71+)	222-D (18-)		
		93	2221-T(64+)	1222-T(10-)		
		80	1222-T(74+)	2221-T(15+)		

Calculated frequencies higher than 2000 cm^{-1}
2213 2213 2212 2212 2176 2163 2152 2124 2113 2100
2076 2076

* Weight of the observed frequency is zero.

Reference

[1] IR.R. I. Harada, H. Takeuchi, M. Sakakibara, H. Matsuura, and T. Shimanouchi, Bull. Chem. Soc. Jpn., **50**, 102 (1977).

No. 8
Molecule: 1'2'2'2'1'-GG $CD_3CD_2CD_2CD_2CD_3$ (gauche-gauche form)
Symmetry C_2 Symmetry number $\sigma = 2$

Sym. species	Observed frequency cm^{-1}	Calculated frequency cm^{-1}	Assignment (P.E.D. %)			
a	1184*	1191	1222-S(19+)	2221-S(19+)	221-5 (17-)	122-5 (17+)
	1142*	1140	221-2 (19-)	122-2 (19-)	222-2 (17-)	2210-S(14-)
	1057*	1057	012-2 (35+)	210-2 (35+)	222-2 (11-)	
	1049*(s)	1052	222-2 (33+)	221-2 (20-)	122-2 (20-)	
	1049*(s)	1046	210-7 (41+)	012-7 (41+)		
	1049*(s)	1044	012-4 (39+)	210-4 (39+)		
	968*	974	012-8 (13+)	210-8 (13+)	122-4 (12-)	221-4 (12+)
	942*	940	222-6 (26+)	210-5 (6+)	012-5 (6+)	221-2 (6+)
		917	122-6 (18+)	221-6 (18+)	222-2 (11+)	222-D (5+)
	802	798	222-6 (23-)	2210-S(14-)	0122-S(14-)	122-5 (6-)
	764*	760	222-6 (32-)	221-5 (19-)	122-5 (19+)	210-5 (8+)
	692*	686	1222-S(18+)	2221-S(18+)	012-5 (12+)	210-5 (12+)
	592	595	210-8 (25-)	012-8 (25-)	122-4 (17-)	221-4 (17+)
	397*	394	222-D (36+)	122-D (22-)	221-D (22-)	
		220	222-D (28-)	221-D (22-)	122-D (22-)	2210-T(10-)
		139	2210-T(37+)	0122-T(37+)	222-D (16-)	
		62	2221-T(46+)	1222-T(46+)		
b		1213	2221-S(42-)	1222-S(42+)	222-5 (22-)	
	1156	1168	0122-S(23-)	2210-S(23+)	122-5 (13+)	221-5 (13+)
	1057*	1060	222-5 (16-)	122-2 (15-)	221-2 (15+)	012-2 (8-)
	1057*	1055	210-2 (33-)	012-2 (33+)	122-2 (17-)	221-2 (17+)
	1049*(s)	1046	012-7 (22+)	210-7 (22-)	210-4 (18-)	012-4 (18+)
	1036*	1040	210-4 (20+)	012-4 (20-)	210-7 (18-)	012-7 (18+)
	968*	973	222-4 (10-)	210-8 (8+)	012-8 (8-)	221-4 (8+)
	953*	956	221-6 (18-)	122-6 (18+)	222-4 (8+)	210-8 (5+)
	881*	885	2210-S(12+)	0122-S(12-)	221-5 (9-)	122-5 (9-)
	753*	759	222-5 (39-)	221-6 (13+)	122-6 (13-)	210-8 (7+)
	723*	723	012-5 (16+)	210-5 (16-)	2221-S(10-)	1222-S(10+)
	659	651	222-4 (39-)	210-5 (10-)	012-5 (10+)	221-5 (10+)
	542*	547	221-4 (32+)	122-4 (32+)	210-8 (15-)	012-8 (15+)
		310	122-D (36-)	221-D (36+)	222-4 (15+)	
		172	0122-T(40-)	2210-T(40+)		
		107	1222-T(34+)	2221-T(34-)	222-4 (9-)	

Calculated frequencies higher than 2000 cm^{-1}
2213 2213 2213 2212 2171 2167 2156 2120 2111 2105
2076 2076

* Weight of the observed frequency is zero.

Reference

[1] IR.R. I. Harada, H. Takeuchi, M. Sakakibara, H. Matsuura, and T. Shimanouchi, Bull. Chem. Soc. Jpn., **50**, 102 (1977).

No. 9
Molecule: 122221-TTT $CH_3CH_2CH_2CH_2CH_2CH_3$ (trans-trans-trans form)
Symmetry C_{2h} Symmetry number $\sigma = 2$

Sym. species	Observed frequency cm^{-1}	Calculated frequency cm^{-1}	Assignment (P.E.D. %)			
a_g	1489	1484	221-2 (27+)	122-2 (27+)	222-2 (10-)	222-2 (10-)
	1457	1457	012-4 (31+)	210-4 (31+)	222-2 (12+)	222-2 (12+)
	1438	1444	222-2 (26+)	222-2 (26+)	221-2 (19+)	122-2 (19+)
	1380	1380	210-2 (49+)	012-2 (49+)		
	1365	1371	222-5 (30-)	222-5 (30+)	2222-S(13-)	122-5 (13+)
	1302	1306	221-5 (29+)	122-5 (29-)	222-5 (16-)	222-5 (16+)
	1143	1147	210-5 (12+)	012-5 (12+)	1222-S(10-)	2221-S(10-)
	1065	1062	2222-S(44+)	2221-S(14-)	1222-S(14-)	
	1007	1012	2210-S(37-)	0122-S(37-)	2222-S(23+)	
	900(s)	903	012-5 (25-)	210-5 (25-)	1222-S(12-)	2221-S(12-)
	372	370	222-D (29+)	222-D (29+)	2221-S(7+)	1222-S(7+)
	305	300	221-D (44+)	122-D (44+)	2222-S(10+)	
a_u	1463(s)	1463	210-7 (41+)	012-7 (41+)		
	1306	1299	221-6 (27+)	122-6 (27+)	222-6 (12-)	222-6 (12-)
	1221	1224	222-6 (16+)	222-6 (16+)	012-8 (10-)	210-8 (10-)
	1000	999	222-6 (24+)	222-6 (24+)	122-6 (15+)	221-6 (15+)
	802	799	122-4 (18-)	221-4 (18+)	210-8 (17-)	012-8 (17-)
	725	725	222-4 (30+)	222-4 (30-)	221-4 (16-)	122-4 (16+)
		236	0122-T(44+)	2210-T(44+)		
		111	2222-T(70+)	1222-T(9+)		
		72	2221-T(35+)	1222-T(35+)	2222-T(13-)	
b_g	1466(s)	1463	012-7 (41-)	210-7 (41+)		
	1302	1305	222-6 (33+)	222-6 (33-)	122-6 (8-)	
	1280	1273	221-6 (28+)	122-6 (28-)	222-6 (7-)	222-6 (7+)
	1178	1176	222-4 (15+)	222-4 (15+)	221-4 (13+)	122-4 (13+)
	899	896	210-8 (22-)	012-8 (22+)	222-4 (17+)	222-4 (17+)
	739(s)	741	122-4 (33+)	221-4 (33+)	222-4 (9-)	
		225	2210-T(48-)	0122-T(48+)		
		150	2221-T(46+)	1222-T(46-)		
b_u	1475(s)	1484	222-2 (25+)	222-2 (25-)	122-2 (14-)	221-2 (14+)
	1463(s)	1468	222-2 (24+)	222-2 (24-)	122-2 (16+)	221-2 (16-)
	1452(s)	1452	210-4 (28-)	012-4 (28+)	122-2 (18-)	221-2 (18+)
	1378	1379	012-2 (52-)	210-2 (52+)		
	1353	1350	221-5 (34-)	122-5 (34-)	222-5 (10+)	222-5 (10+)
	1246	1246	222-5 (35+)	222-5 (35+)	221-5 (6+)	
	1065	1068	1222-S(22+)	2221-S(22-)	122-5 (9-)	221-5 (9-)
	1037	1040	0122-S(33+)	2210-S(33-)	210-5 (9+)	
	884	885	2221-S(22-)	1222-S(22+)	210-5 (16-)	012-5 (16+)
	468	476	122-D (30-)	221-D (30+)	222-D (12-)	222-D (12+)
		137	222-D (44+)	222-D (44-)	221-D (18-)	122-D (18+)

Calculated frequencies higher than 2000 cm^{-1}
2962 2962 2962 2962 2912 2907 2902 2898 2880 2880
2876 2871 2866 2863

References

[1] IR. R. G. Snyder and J. H. Schachtschneider, Spectrochim. Acta, **19**, 85 (1963).
[2] IR. R. G. Snyder, J. Chem. Phys., **47**, 1316 (1967).
[3] R. I. Harada, H. Takeuchi, M. Sakakibara, H. Matsuura, and T. Shimanouchi, Bull. Chem. Soc. Jpn., **50**, 102 (1977).

No. 10
Molecule: 122221-TTG $CH_3CH_2CH_2CH_2CH_2CH_3$ (trans-trans-gauche form)
Symmetry C_1 Symmetry number $\sigma = 1$

Sym. species	Observed frequency cm^{-1}	Calculated frequency cm^{-1}	Assignment (P.E.D. %)			
a	1489*	1485	222-2 (28-)	222-2 (25+)	221-2 (24-)	
	1475*(s)	1483	122-2 (35-)	221-2 (21+)	012-4 (11-)	222-2 (10+)
	1466*(s)	1473	222-2 (29+)	210-4 (22-)	221-2 (18-)	122-2 (9-)
	1463*(s)	1463	210-7 (76+)	210-8 (13+)		
	1463*(s)	1463	012-7 (81+)	012-8 (14+)		
	1457*	1457	012-4 (38-)	222-2 (30-)	210-4 (12+)	
	1452*(s)	1454	210-4 (40+)	221-2 (22-)	012-4 (15+)	
	1438*	1447	122-2 (32+)	222-2 (21+)	222-2 (20+)	012-4 (12-)
	1380	1381	210-2 (82+)	012-2 (11+)		
	1378	1379	012-2 (91-)	210-2 (14+)		
	1365	1369	222-5 (34-)	222-5 (25+)	122-5 (18+)	2222-S(12-)
	1343	1345	221-5 (66+)	2210-S(7+)		
	1330	1334	122-5 (40-)	222-5 (33+)		
	1302	1303	222-6 (47+)	122-6 (23-)	222-6 (11-)	
	1280	1285	122-6 (26-)	222-6 (24+)	221-6 (13+)	222-5 (8+)
	1280	1273	221-6 (29+)	222-5 (18+)	122-6 (14+)	122-5 (6+)
	1250	1252	222-5 (26+)	221-6 (17-)	222-5 (17+)	210-8 (9+)
	1222	1219	222-6 (22+)	222-6 (16+)	012-8 (13-)	122-4 (12+)
	1167	1166	222-4 (13-)	222-4 (11-)	210-5 (8+)	122-4 (8-)
	1136	1139	012-5 (12-)	1222-S(11+)	2222-S(10+)	210-5 (8+)
	1080	1087	2221-S(23-)	2222-S(20+)	2210-S(16+)	221-5 (7-)
	1057	1057	1222-S(29-)	0122-S(14+)	2210-S(11-)	2221-S(10+)
	1039	1035	0122-S(47-)	012-5 (11+)	210-8 (7-)	222-5 (7+)
	1007	1007	222-6 (19-)	222-6 (19-)	210-5 (18+)	2210-S(13-)
	975	976	2222-S(33-)	0122-S(16+)	221-6 (10-)	210-8 (9-)
	899	901	012-8 (22+)	222-4 (18+)	122-6 (16+)	222-4 (16+)
	891	896	012-5 (36-)	1222-S(24-)	210-8 (10-)	122-5 (9-)
	870	877	2221-S(32-)	2210-S(29-)	210-5 (14-)	
	794	795	222-4 (20+)	221-4 (18-)	122-4 (15-)	012-8 (14-)
	758	758	221-4 (38+)	122-4 (20-)	210-8 (17-)	222-4 (11+)
	727	728	222-4 (40-)	122-4 (31+)	222-4 (14+)	
	456	456	221-D (38+)	222-D (34-)		
	402	402	122-D (45-)	222-D (19-)	2222-S(8-)	
	320	319	221-D (43+)	222-D (12+)	222-D (11+)	2221-T(6-)
		234	2210-T(61-)	222-D (18+)	122-D (16-)	
		230	0122-T(92+)			
		170	2210-T(26-)	222-D (23-)	222-D (19+)	2221-T(19-)
		134	1222-T(46-)	2221-T(18+)	222-D (15+)	
		90	2222-T(77+)			
		80	2221-T(37-)	1222-T(36-)		

Calculated frequencies higher than 2000 cm^{-1}

2963 2963 2962 2962 2911 2906 2904 2899 2880 2880
2875 2870 2868 2864

* Weight of the observed frequency is zero.

References

[1] IR. R. G. Snyder, J. Chem. Phys., 47, 1316 (1967).
[2] R. I. Harada, H. Takeuchi, M. Sakakibara, H. Matsuura, and T. Shimanouchi, Bull. Chem. Soc. Jpn., **50**, 102 (1977).

No. 11
Molecule: 122221-TGT $CH_3CH_2CH_2CH_2CH_2CH_3$ **(trans-gauche-trans form)**
Symmetry C_2 **Symmetry number** $\sigma = 2$

Sym. species	Observed frequency cm^{-1}	Calculated frequency cm^{-1}	Assignment (P.E.D. %)			
a	1489*	1491	222-2 (27+)	222-2 (27+)	122-2 (14-)	221-2 (14-)
	1466*(s)	1467	222-2 (19+)	222-2 (19+)	122-2 (13+)	221-2 (13+)
	1463*(s)	1463	012-7 (40+)	210-7 (40+)		
	1452*(s)	1452	012-4 (26+)	210-4 (26+)	122-2 (20-)	221-2 (20-)
	1380	1379	012-2 (52+)	210-2 (52+)		
	1365	1361	221-5 (23-)	122-5 (23+)	222-5 (18+)	222-5 (18-)
	1306	1302	222-6 (22+)	222-6 (22+)	122-5 (10+)	221-5 (10-)
	1287	1292	122-6 (20+)	221-6 (20+)	222-5 (11-)	222-5 (11+)
	1234	1240	222-6 (13+)	222-6 (13+)	222-5 (8-)	222-5 (8+)
	1167	1162	222-4 (10+)	222-4 (10-)	221-4 (8+)	122-4 (8-)
	1080	1086	2222-S(36-)	2221-S(18+)	1222-S(18+)	
	1039	1038	012-5 (14+)	210-5 (14+)	0122-S(10-)	2210-S(10-)
	1007	1011	2210-S(29+)	0122-S(29+)	2222-S(25-)	
	899	900	012-8 (15-)	210-8 (15-)	222-4 (13-)	222-4 (13+)
	824	824	1222-S(18+)	2221-S(18+)	210-5 (10+)	012-5 (10+)
	746	745	122-4 (30+)	221-4 (30-)	222-4 (10-)	222-4 (10+)
	332	333	221-D (22+)	122-D (22+)	2222-S(12+)	222-D (9+)
		259	122-D (16-)	221-D (16-)	2222-T(15-)	222-D (14+)
		222	2210-T(34+)	0122-T(34+)	222-D (7-)	
		103	2222-T(66-)	2221-T(12-)	1222-T(12-)	
		89	2221-T(25+)	1222-T(25+)	222-D (12-)	222-D (12-)
b	1475*(s)	1481	221-2 (25+)	122-2 (25-)	210-4 (10+)	012-4 (10-)
	1463*(s)	1463	012-7 (40+)	210-7 (40-)		
	1457*	1457	222-2 (29-)	222-2 (29+)	210-4 (17-)	012-4 (17+)
	1452*(s)	1451	221-2 (23-)	122-2 (23+)	210-4 (15+)	012-4 (15-)
	1378	1380	210-2 (51-)	012-2 (51+)		
	1365	1367	222-5 (26-)	222-5 (26-)	122-5 (16+)	221-5 (16+)
	1302	1300	221-5 (25+)	122-5 (25+)	222-5 (16+)	222-5 (16+)
	1293	1296	221-6 (27+)	122-6 (27-)	222-6 (13+)	222-6 (13-)
	1222	1228	222-6 (17+)	222-6 (17-)	012-8 (9+)	210-8 (9-)
	1143	1142	210-5 (10-)	012-5 (10+)	2221-S(10+)	1222-S(10-)
	1033	1033	0122-S(37-)	2210-S(37+)	1222-S(10+)	2221-S(10-)
	1013	1014	222-6 (17+)	222-6 (17-)	012-8 (9+)	210-8 (9-)
	904	903	012-5 (18+)	210-5 (18-)	1222-S(12+)	2221-S(12-)
	811	819	012-8 (14+)	210-8 (14-)	222-4 (13+)	222-4 (13+)
	727	727	221-4 (25+)	122-4 (25+)	222-4 (18-)	222-4 (18-)
	520	517	222-D (20-)	222-D (20+)	122-D (14-)	221-D (14+)
	294	298	122-D (32-)	221-D (32+)	222-D (23-)	222-D (23+)
		227	0122-T(47+)	2210-T(47-)		
		82	1222-T(42+)	2221-T(42-)		

Calculated frequencies higher than 2000 cm^{-1}

2962 2962 2962 2962 2910 2908 2902 2900 2880 2880
2873 2872 2866 2864

* Weight of the observed frequency is zero.

References

[1] IR. R. G. Snyder, J. Chem. Phys., 47, 1316 (1967).
[2] R. I. Harada, H. Takeuchi, M. Sakakibara, H. Matsuura, and T. Shimanouchi, Bull. Chem. Soc. Jpn., 50, 102 (1977).

No. 12
Molecule: 122221-TGG $CH_3CH_2CH_2CH_2CH_2CH_3$ (trans-gauche-gauche form)
Symmetry C_1 Symmetry number $\sigma = 1$

Sym. species	Observed frequency cm^{-1}	Calculated frequency cm^{-1}	Assignment (P.E.D. %)			
a	1489*	1492	222-2 (31+)	222-2 (29+)	221-2 (13+)	122-2 (13-)
	1475*(s)	1481	221-2 (34+)	122-2 (25+)	012-4 (10+)	222-2 (7-)
	1466*(s)	1472	222-2 (28-)	210-4 (22+)	221-2 (15+)	122-2 (11-)
	1463*(s)	1463	210-7 (61+)	012-7 (16-)	210-8 (11+)	
	1463*(s)	1463	012-7 (65+)	210-7 (14+)	012-8 (11+)	
	1457*	1459	222-2 (41+)	012-4 (21+)	210-4 (13+)	222-2 (10-)
	1452*(s)	1452	210-4 (39-)	221-2 (25+)	222-2 (12-)	
	1452*(s)	1451	122-2 (40+)	012-4 (33-)	222-2 (10+)	
	1380*	1381	210-2 (95+)			
	1378*	1379	012-2 (97+)			
	1365*	1366	222-5 (41-)	122-5 (31+)	1222-S(14+)	
	1353*	1353	222-5 (46+)	221-5 (18+)	2222-S(10-)	122-5 (10+)
	1343*	1342	221-5 (53+)	2221-S(16-)	222-5 (14-)	
	1302*	1301	122-5 (29+)	222-5 (17+)	222-6 (15+)	222-6 (12+)
	1293*	1294	122-6 (41-)	122-5 (12-)	222-6 (12+)	222-5 (11-)
	1280*	1273	221-6 (47+)	222-6 (10+)	210-8 (5-)	210-7 (4+)
	1246*	1241	222-6 (15+)	222-6 (11+)	221-6 (9-)	122-6 (8+)
	1222*	1219	222-6 (26-)	222-6 (15+)	012-8 (10-)	122-4 (9+)
	1152	1151	222-4 (13+)	210-5 (11-)	012-5 (11+)	2221-S(10+)
	1143*	1140	222-4 (11-)	221-4 (9+)	222-D (7+)	210-8 (7+)
	1088	1100	2221-S(18-)	2210-S(16+)	2222-S(16+)	1222-S(12-)
	1039*	1037	0122-S(58-)	012-5 (9+)	222-5 (7+)	
	1033*	1033	1222-S(13+)	210-8 (13-)	221-6 (11-)	222-5 (11+)
	1013*	1013	2210-S(30+)	222-6 (15-)	210-5 (11-)	222-6 (10+)
	975*	975	2222-S(32+)	2210-S(15-)	0122-S(13-)	210-5 (12-)
	904*	906	012-5 (23-)	222-4 (19+)	210-5 (13+)	1222-S(12-)
	891*	891	222-4 (21+)	012-8 (21+)	2210-S(17+)	122-6 (15+)
	824*	828	1222-S(24-)	210-8 (16-)	222-4 (13-)	221-4 (12+)
	811*	817	2221-S(29-)	012-8 (12+)	2210-S(10-)	222-4 (9+)
	758*	760	122-4 (28+)	221-4 (26+)	210-8 (13-)	012-8 (11+)
	727*	724	122-4 (30-)	222-4 (29+)	221-4 (16+)	222-4 (11+)
	488	493	222-D (37+)	222-D (20-)	221-D (14-)	
	402*	398	221-D (45+)	122-D (12-)	222-D (11-)	222-4 (7+)
	311	312	122-D (49+)	222-D (16+)	221-D (11+)	
		241	0122-T(35+)	222-D (21+)	122-D (11-)	221-D (10+)
		229	0122-T(41+)	2210-T(40-)	222-D (11-)	
		205	2210-T(34-)	0122-T(16-)	222-D (16+)	221-D (10+)
		129	2221-T(38+)	2222-T(18-)	222-D (13-)	222-4 (9+)
		92	1222-T(61+)	2222-T(28+)		
		61	2221-T(41-)	2222-T(30-)	1222-T(12+)	

Calculated frequencies higher than 2000 cm^{-1}

2963 2963 2962 2962 2910 2908 2904 2900 2880 2880
2873 2870 2867 2865

* Weight of the observed frequency is zero.

References

[1] IR. R. G. Snyder, J. Chem. Phys., **47**, 1316 (1967).
[2] R. I. Harada, H. Takeuchi, M. Sakakibara, H. Matsuura, and T. Shimanouchi, Bull. Chem. Soc. Jpn., **50**, 102 (1977).

No. 13

Molecule: 122221-GTG $CH_3CH_2CH_2CH_2CH_2CH_3$ (gauche-trans-gauche form)

Symmetry C_2 Symmetry number $\sigma = 2$

Sym. species	Observed frequency cm^{-1}	Calculated frequency cm^{-1}	Assignment (P.E.D. %)			
a	1475*(s)	1481	221-2 (31+)	122-2 (31+)	210-4 (7+)	012-4 (7+)
	1466*(s)	1465	210-7 (26+)	012-7 (26+)	222-2 (11+)	222-2 (11+)
	1457*	1460	222-2 (15-)	222-2 (15-)	210-4 (15+)	012-4 (15+)
	1452*(s)	1451	012-4 (16-)	210-4 (16-)	222-2 (15-)	222-2 (15-)
	1380*	1382	012-2 (45+)	210-2 (45+)		
	1365*	1367	222-5 (34+)	222-5 (34-)	2222-S(12+)	
	1343*	1343	221-5 (34+)	122-5 (34-)	2221-S(7-)	
	1280*	1272	122-6 (29+)	221-6 (29+)	012-8 (4-)	210-8 (4-)
	1215	1213	222-6 (23+)	222-6 (23+)	012-5 (4+)	210-5 (4+)
	1136*	1134	2222-S(14-)	122-4 (9-)	221-4 (9+)	012-8 (7+)
	1088	1097	1222-S(17-)	2221-S(17-)	2222-S(15+)	0122-S(9+)
	1007*	1012	222-6 (17-)	222-6 (17-)	012-5 (15+)	210-5 (15+)
	952	946	2222-S(36+)	0122-S(9-)	2210-S(9-)	210-5 (7-)
	891*	881	210-8 (11+)	012-8 (11+)	0122-S(10+)	2210-S(10+)
	794*	782	222-4 (22+)	222-4 (22-)	122-4 (11+)	221-4 (11-)
	727*	731	222-4 (19+)	222-4 (19-)	221-4 (17-)	122-4 (17+)
	488	488	221-D (19+)	122-D (19+)	222-D (17-)	222-D (17-)
	305*	308	221-D (20-)	122-D (20-)	222-D (9-)	222-D (9-)
		211	2210-T(41-)	0122-T(41-)		
		96	1222-T(32+)	2221-T(32+)	2222-T(11-)	
		62	2222-T(69-)	1222-T(11-)	2221-T(11-)	
b	1489*	1487	222-2 (28+)	222-2 (28-)	122-2 (18+)	221-2 (18-)
	1475*(s)	1474	222-2 (16-)	222-2 (16+)	122-2 (14+)	221-2 (14-)
	1463*(s)	1463	012-7 (40+)	210-7 (40-)		
	1452*(s)	1453	012-4 (27-)	210-4 (27+)	221-2 (14-)	122-2 (14+)
	1378*	1380	210-2 (53+)	012-2 (53-)		
	1343*	1345	122-5 (38+)	221-5 (38+)		
	1315	1306	222-5 (21+)	222-5 (21+)	122-6 (12-)	221-6 (12+)
	1287*	1288	222-6 (27+)	222-6 (27-)	222-5 (8+)	222-5 (8+)
	1250*	1254	221-6 (19+)	122-6 (19-)	222-5 (9-)	222-5 (9-)
	1152	1150	222-4 (14+)	222-4 (14+)	012-5 (12+)	210-5 (12-)
	1057*	1059	2221-S(18-)	1222-S(18+)	2210-S(17+)	0122-S(17-)
	1039*	1031	012-8 (13-)	210-8 (13+)	222-5 (11-)	222-5 (11-)
	904*	906	222-4 (18+)	222-4 (18+)	012-5 (15-)	210-5 (15+)
	870*	877	2210-S(18+)	0122-S(18-)	2221-S(17+)	1222-S(17-)
	772	774	221-4 (31+)	122-4 (31+)	210-8 (17-)	012-8 (17+)
	372*	385	122-D (39-)	221-D (39+)		
	294*	287	222-D (21+)	222-D (21-)	0122-T(18+)	2210-T(18-)
		185	0122-T(29-)	2210-T(29+)	222-D (16+)	222-D (16-)
		130	2221-T(34-)	1222-T(34+)	222-D (11+)	222-D (11-)

Calculated frequencies higher than 2000 cm^{-1}

2963 2962 2962 2962 2910 2906 2904 2900 2880 2880

2873 2869 2868 2865

* Weight of the observed frequency is zero.

References

[1] IR. R. G. Snyder, J. Chem. Phys., **47**, 1316 (1967).

[2] R. I. Harada, H. Takeuchi, M. Sakakibara, H. Matsuura, and T. Shimanouchi, Bull. Chem. Soc. Jpn., **50**, 102 (1977).

No. 14
Molecule: 122221-GTG′ $CH_3CH_2CH_2CH_2CH_2CH_3$ (gauche-trans-gauche′ form)
Symmetry C_i Symmetry number $\sigma = 1$

Sym. species	Observed frequency cm^{-1}	Calculated frequency cm^{-1}	Assignment (P.E.D. %)			
a_g	1489*	1481	221-2 (31+)	122-2 (31+)	210-4 (7+)	012-4 (7+)
	1457*	1465	210-7 (26+)	012-7 (26-)	222-2 (11-)	222-2 (11-)
	1457*	1460	222-2 (15-)	222-2 (15-)	210-4 (15+)	012-4 (15+)
	1450*	1452	012-4 (16+)	210-4 (16+)	222-2 (15+)	222-2 (15+)
	1380*	1382	210-2 (45+)	012-2 (45+)		
	1365*	1367	222-5 (33+)	222-5 (33-)	2222-S(12+)	
	1343*	1343	221-5 (34+)	122-5 (34-)	2221-S(8-)	
	1302*	1294	222-6 (35-)	222-6 (35+)	222-4 (2+)	
		1267	122-6 (30-)	221-6 (30+)	012-8 (5+)	210-8 (5-)
	1167*	1167	222-4 (10+)	222-4 (10+)	221-4 (9-)	122-4 (9-)
		1127	2222-S(19+)	012-5 (8+)	210-5 (8+)	122-4 (4+)
	1080*	1086	0122-S(19+)	2210-S(19+)	1222-S(14-)	2221-S(14-)
	952	949	2222-S(36-)	012-5 (14+)	210-5 (14+)	221-5 (7-)
	899*	902	222-4 (18-)	222-4 (18-)	210-8 (9-)	012-8 (9+)
	870*	878	2210-S(18+)	0122-S(18+)	2221-S(9+)	1222-S(9+)
	746*	748	221-4 (29+)	122-4 (29+)	2222-S(14-)	210-8 (11-)
	488*	478	222-D (20+)	222-D (20+)	221-D (17-)	122-D (17-)
	305*	294	221-D (22+)	122-D (22+)	2221-T(9+)	1222-T(9-)
		210	2210-T(40+)	0122-T(40-)		
		135	1222-T(39+)	2221-T(39-)		
a_u	1475*(s)	1487	222-2 (29+)	222-2 (29-)	122-2 (17+)	221-2 (17-)
	1475*(s)	1473	222-2 (15-)	222-2 (15+)	122-2 (14+)	221-2 (14-)
	1463*(s)	1463	012-7 (40+)	210-7 (40+)		
	1452*(s)	1453	210-4 (27-)	012-4 (27+)	221-2 (15+)	122-2 (15-)
	1378*	1380	012-2 (53+)	210-2 (53-)		
	1343*	1345	122-5 (36+)	221-5 (36+)		
	1306*	1304	222-5 (28+)	222-5 (28+)	122-6 (15-)	221-6 (15-)
	1253*	1255	221-6 (18-)	122-6 (18-)	222-5 (10-)	222-5 (10-)
	1215	1208	222-6 (26-)	222-6 (26-)	012-5 (6-)	210-5 (6+)
	1065*	1068	2221-S(19-)	1222-S(19+)	2210-S(9+)	0122-S(9-)
	1033*	1031	012-8 (11+)	210-8 (11+)	222-5 (11+)	222-5 (11+)
	1004*	1007	222-6 (17+)	222-6 (17+)	0122-S(14+)	2210-S(14-)
	884*	881	1222-S(20+)	2221-S(20-)	012-5 (14+)	210-5 (14-)
	802*	801	122-4 (19+)	221-4 (19-)	210-8 (15+)	012-8 (15+)
	744*	739	222-4 (30-)	222-4 (30+)	122-4 (12-)	221-4 (12+)
	402*	409	122-D (39+)	221-D (39-)		
	294*	287	222-D (24+)	222-D (24-)	0122-T(21+)	2210-T(21+)
		182	0122-T(27+)	2210-T(27+)	222-D (21-)	222-D (21+)
		91	2222-T(26-)	1222-T(22+)	2221-T(22+)	222-4 (8-)
		62	2222-T(55+)	2221-T(19+)	1222-T(19+)	

Calculated frequencies higher than 2000 cm^{-1}

2963 2962 2962 2962 2910 2906 2905 2900 2880 2880
2873 2869 2868 2865

* Weight of the observed frequency is zero.

References

[1] IR. R. G. Snyder, J. Chem. Phys., **47**, 1316 (1967).
[2] R. I. Harada, H. Takeuchi, M. Sakakibara, H. Matsuura, and T. Shimanouchi, Bull. Chem. Soc. Jpn., **50**, 102 (1977).

No. 15

Molecule: **1′2′2′2′2′1′-TTT** $CD_3CD_2CD_2CD_2CD_2CD_3$ **(trans-trans-trans form)**

Symmetry C_{2h} **Symmetry number $\sigma = 2$**

Sym. species	Observed frequency cm^{-1}	Calculated frequency cm^{-1}	Assignment (P.E.D. %)			
a_g	1246	1244	2222-S(40-)	1222-S(23+)	2221-S(23+)	222-5 (19-)
	1152	1143	0122-S(26+)	2210-S(26+)	122-2 (13+)	221-2 (13+)
	1130	1129	222-2 (23+)	222-2 (23+)	2222-S(18+)	1222-S(9+)
	1057	1064	221-2 (18+)	122-2 (18+)	221-5 (12-)	122-5 (12+)
	1053(s)	1054	210-2 (36+)	012-2 (36+)		
	1045(s)	1042	210-4 (35-)	012-4 (35-)	210-5 (6-)	
	975	965	222-2 (14-)	222-2 (14-)	122-2 (7-)	221-2 (7-)
	873	871	2222-S(14+)	2210-S(14-)	0122-S(14-)	222-2 (7-)
	839	832	222-5 (14+)	222-5 (14-)	2222-S(12-)	122-5 (8-)
	709	705	210-5 (29-)	012-5 (29-)	221-5 (11+)	122-5 (11-)
	335	331	222-D (27+)	222-D (27+)	1222-S(7+)	2221-S(7+)
	263	261	122-D (43+)	221-D (43+)		
a_u	1054(s)	1046	210-7 (40+)	012-7 (40+)		
	981	980	221-4 (13+)	122-4 (13-)	222-6 (12-)	222-6 (12-)
	960(s)	954	122-6 (28+)	221-6 (28+)	210-8 (6-)	012-8 (6-)
	726(s)	725	222-6 (33+)	222-6 (33+)	221-6 (17+)	122-6 (17+)
	595	593	012-8 (20+)	210-8 (20+)	122-4 (14+)	221-4 (14-)
	524	525	222-4 (29+)	222-4 (29-)	221-4 (16-)	122-4 (16+)
		175	0122-T(42+)	2210-T(42+)	2222-T(13-)	
		87	2222-T(70+)	1222-T(6+)		
		62	2221-T(38-)	1222-T(38-)		
b_g	1045(s)	1046	012-7 (40+)	210-7 (40-)		
	991	990	222-4 (22+)	222-4 (22+)	122-4 (9+)	221-4 (9+)
	975	971	122-6 (11-)	221-6 (11+)	210-8 (11-)	012-8 (11+)
	936	932	222-6 (25+)	222-6 (25-)	221-6 (14-)	122-6 (14+)
	665	664	221-6 (22-)	122-6 (22+)	012-8 (20+)	210-8 (20-)
	538(s)	542	221-4 (32+)	122-4 (32+)	210-8 (11-)	012-8 (11+)
		163	2210-T(48-)	0122-T(48+)		
		126	2221-T(47+)	1222-T(47-)		
b_u	1214	1209	2221-S(24+)	1222-S(24-)	221-5 (16-)	122-5 (16-)
	1115	1119	221-2 (17+)	122-2 (17-)	2210-S(11+)	0122-S(11-)
	1090	1081	222-2 (30+)	222-2 (30-)	122-2 (12-)	221-2 (12+)
	1057	1055	012-2 (37-)	210-2 (37+)	122-2 (10+)	221-2 (10-)
	1054(s)	1044	012-4 (40+)	210-4 (40-)		
	987	986	222-5 (26+)	222-5 (26+)	012-5 (8-)	210-5 (8+)
	892	884	0122-S(15+)	2210-S(15-)	222-5 (12-)	222-5 (12-)
	856	850	221-5 (18-)	122-5 (18-)	2221-S(11-)	1222-S(11+)
	719	714	012-5 (24+)	210-5 (24-)	1222-S(7+)	2221-S(7-)
	405	409	122-D (26-)	221-D (26+)	222-D (12-)	222-D (12+)
		120	222-D (43+)	222-D (43-)	122-D (18+)	221-D (18-)

Calculated frequencies higher than 2000 cm^{-1}

2213 2213 2212 2212 2181 2168 2155 2146 2133 2119
2105 2096 2076 2075

Reference

[1] IR.R. I. Harada, H. Takeuchi, M. Sakakibara, H. Matsuura, and T. Shimanouchi, Bull. Chem. Soc. Jpn., **50**, 102 (1977).

No. 16
Molecule: 1′2′2′2′2′1′-TTG $CD_3CD_2CD_2CD_2CD_2CD_3$ (trans-trans-gauche form)
Symmetry C_1 Symmetry number $\sigma = 1$

Sym. species	Observed frequency cm^{-1}	Calculated frequency cm^{-1}	Assignment (P.E.D. %)			
a	1241	1242	2222-S(40-)	1222-S(31+)	222-5 (23-)	2221-S(16+)
	1201	1198	2221-S(41+)	221-5 (18-)	0122-S(14+)	2210-S(13-)
	1166	1169	2210-S(29+)	221-5 (18+)	0122-S(11+)	2222-S(9-)
	1138	1134	222-2 (23+)	221-2 (22+)	2210-S(11+)	2222-S(10+)
	1130	1125	122-2 (26-)	0122-S(21-)	222-2 (16-)	1222-S(13-)
	1080	1082	222-2 (37+)	122-2 (24-)	222-2 (13-)	
	1057	1060	222-2 (21+)	210-2 (19-)	221-5 (14+)	221-2 (12-)
	1057	1055	210-2 (58+)	221-2 (24-)	012-2 (12+)	
	1057	1054	012-2 (57-)	122-2 (11+)	221-2 (10-)	
	1042	1046	210-7 (70+)	210-8 (12+)		
	1042	1046	012-7 (80+)	012-8 (13+)		
	1042	1045	210-4 (59-)	012-4 (20+)		
	1042	1042	012-4 (49+)	210-4 (19+)	012-5 (7+)	
	1004*	1007	222-5 (31+)	222-5 (15+)	122-5 (10+)	012-5 (9-)
	987	988	222-4 (25-)	122-4 (15-)	222-4 (13-)	222-6 (9-)
	975	975	222-6 (19-)	012-8 (12+)	122-4 (11-)	012-7 (7-)
	964	968	210-8 (12+)	221-6 (10-)	122-6 (10-)	222-6 (7+)
	951	952	221-6 (26-)	122-6 (17+)	210-8 (7+)	222-6 (6-)
	951	949	222-2 (10+)	122-6 (7+)	210-5 (7-)	122-2 (6+)
	936	935	222-6 (21-)	222-6 (20+)	122-6 (15+)	210-5 (6+)
	880	876	0122-S(15+)	2210-S(11+)	221-5 (10-)	2221-S(9-)
	873	869	0122-S(15-)	2222-S(11+)	222-5 (10+)	222-2 (9-)
	839	838	122-5 (22+)	1222-S(15-)	222-5 (11-)	2222-S(8+)
	760	762	221-5 (22+)	221-6 (16+)	222-5 (12-)	210-5 (10-)
	752	756	222-6 (30+)	2210-S(17+)	222-6 (9+)	221-6 (9-)
	719	717	210-5 (23-)	222-6 (11+)	2221-S(11-)	122-6 (6+)
	709	704	012-5 (44-)	122-5 (14-)	1222-S(11-)	221-6 (7-)
	665	673	122-6 (26+)	012-8 (21+)	222-4 (16+)	210-5 (12+)
	594	593	210-8 (18+)	012-8 (17-)	222-4 (17+)	221-4 (16-)
	570	569	221-4 (32-)	210-8 (25+)	122-4 (12+)	222-4 (11-)
	532	531	222-4 (39-)	122-4 (39+)		
	385	385	221-D (29-)	222-D (29+)	221-4 (9-)	210-5 (8+)
	350	352	122-D (44-)	222-D (18-)	012-5 (9+)	
	270	269	221-D (47-)	222-D (10-)	222-D (10-)	122-D (7+)
		185	2210-T(44+)	222-D (24-)	122-D (21+)	
		168	0122-T(91-)			
		131	2210-T(47+)	222-D (15-)	222-D (14+)	2221-T(13+)
		114	1222-T(44-)	2221-T(21+)	222-D (14+)	
		73	2222-T(80+)			
		67	2221-T(46+)	1222-T(38+)		

Calculated frequencies higher than 2000 cm^{-1}

2213 2213 2212 2212 2180 2167 2160 2148 2130 2116
2109 2097 2076 2076

* Weight of the observed frequency is zero.

Reference

[1] IR.R. I. Harada, H. Takeuchi, M. Sakakibara, H. Matsuura, and T. Shimanouchi, Bull. Chem. Soc. Jpn., **50**, 102 (1977).

No. 17
Molecule: 1′2′2′2′2′1′-TGT $CD_3CD_2CD_2CD_2CD_2CD_3$ (trans-gauche-trans form)
Symmetry C_2 **Symmetry number** $\sigma = 2$

Sym. species	Observed frequency cm^{-1}	Calculated frequency cm^{-1}	Assignment (P.E.D. %)			
a	1232	1239	2222-S(39-)	1222-S(21+)	2221-S(21+)	222-5 (13-)
	1152	1153	222-2 (23+)	222-2 (23+)	2222-S(21+)	2210-S(6-)
	1130	1125	221-2 (18+)	122-2 (18+)	2210-S(15+)	0122-S(15+)
	1057	1056	122-2 (18-)	221-2 (18-)	012-2 (18+)	210-2 (18+)
	1057	1053	012-2 (17+)	210-2 (17+)	012-4 (13+)	210-4 (13+)
	1042	1046	210-7 (38+)	012-7 (38+)		
	1042	1041	210-4 (27+)	012-4 (27+)	210-5 (7+)	012-5 (7+)
	981	982	122-4 (11+)	221-4 (11-)	222-4 (10+)	222-4 (10-)
	964	966	122-6 (14+)	221-6 (14+)	210-8 (8-)	012-8 (8-)
	936	939	222-6 (14-)	222-6 (14-)	221-6 (13+)	122-6 (13+)
	892	887	2222-S(14+)	0122-S(11-)	2210-S(11-)	222-6 (8-)
	846	849	221-5 (14-)	122-5 (14+)	2221-S(8-)	1222-S(8-)
	771	771	222-5 (20-)	222-5 (20+)	222-6 (10-)	222-6 (10-)
	695	690	210-5 (22+)	012-5 (22+)	2221-S(8+)	1222-S(8+)
	655	649	012-8 (15+)	210-8 (15+)	122-6 (15+)	221-6 (15+)
	540	547	221-4 (30+)	122-4 (30-)	210-8 (11-)	012-8 (11-)
	294	293	122-D (22+)	221-D (22+)	2222-S(11+)	222-D (8+)
		210	222-D (20+)	222-D (20+)	122-D (16-)	221-D (16-)
		167	2210-T(41+)	0122-T(41+)		
		82	2222-T(74+)			
		78	2221-T(34-)	1222-T(34-)	222-D (10+)	222-D (10+)
b	1214	1211	2221-S(28+)	1222-S(28-)	222-5 (13+)	222-5 (13+)
	1130	1134	0122-S(19-)	2210-S(19+)	122-2 (14-)	221-2 (14+)
	1080	1076	222-2 (24+)	222-2 (24-)	221-2 (16+)	122-2 (16-)
	1057	1054	210-2 (35+)	012-2 (35-)	221-2 (8-)	
	1042	1047	012-7 (35-)	210-7 (35+)	012-8 (6-)	
	1042	1043	012-4 (36+)	210-4 (36-)		
	1042	1037	222-5 (21+)	222-5 (21+)	222-2 (7-)	222-2 (7+)
	975	978	221-4 (13+)	122-4 (13+)	222-6 (9-)	222-6 (9+)
	957	954	122-6 (18+)	221-6 (18-)	012-5 (3-)	210-5 (3+)
	951	945	221-6 (10-)	122-6 (10+)	222-6 (7-)	222-6 (7+)
	854	852	0122-S(13+)	2210-S(13-)	122-5 (10+)	221-5 (10+)
	752	748	222-6 (28-)	222-6 (28+)	122-6 (8+)	221-6 (8-)
	709	703	012-5 (23+)	210-5 (23-)	1222-S(10+)	2221-S(10-)
	638	634	210-8 (18-)	012-8 (18+)	222-4 (16+)	222-4 (16+)
	540	540	122-4 (28-)	221-4 (28-)	012-8 (9-)	210-8 (9+)
	438	440	222-D (16-)	222-D (16+)	122-D (12-)	221-D (12+)
		253	221-D (31+)	122-D (31-)	222-D (22+)	222-D (22-)
		165	0122-T(48+)	2210-T(48-)		
		68	1222-T(42+)	2221-T(42-)		

Calculated frequencies higher than 2000 cm^{-1}

2213 2213 2212 2212 2178 2172 2155 2151 2125 2122
2105 2098 2076 2076

Reference

[1] IR.R. I. Harada, H. Takeuchi, M. Sakakibara, H. Matsuura, and T. Shimanouchi, Bull. Chem. Soc. Jpn., **50**, 102 (1977).

No. 18
Molecule: 1′2′2′2′2′1′-TGG $CD_3CD_2CD_2CD_2CD_2CD_3$ (trans-gauche-gauche form)
Symmetry C_1 Symmetry number $\sigma = 1$

Sym. species	Observed frequency cm^{-1}	Calculated frequency cm^{-1}	Assignment (P.E.D. %)			
a	1232*	1232	2222-S(39-)	1222-S(34+)	222-5 (20-)	122-5 (17+)
	1201*	1203	2221-S(51+)	222-5 (15+)	221-5 (14-)	1222-S(11-)
	1179	1178	2210-S(23-)	221-5 (19-)	2222-S(14+)	222-5 (11-)
	1152*	1148	2210-S(21+)	221-2 (20+)	222-2 (17+)	222-2 (7+)
	1130*	1129	0122-S(32+)	122-2 (31+)	012-2 (14+)	
	1080*	1073	222-2 (38-)	122-2 (22+)	222-2 (13+)	122-5 (10+)
	1057*	1059	210-2 (22-)	221-2 (17-)	221-5 (15+)	222-5 (13+)
	1057*	1055	210-2 (61+)	221-2 (34-)		
	1057*	1054	012-2 (72-)	122-2 (17+)		
	1042*	1046	012-7 (69+)	012-8 (11+)		
	1042*	1046	210-7 (48+)	210-4 (27+)		
	1042*	1044	012-4 (61+)	222-2 (9-)	222-2 (6+)	
	1042*	1042	210-4 (49+)	210-7 (23-)		
	1042*	1039	222-5 (24+)	222-2 (19-)	012-5 (13-)	122-5 (12+)
	981*	982	122-4 (25+)	222-4 (15+)	012-8 (12-)	012-7 (11+)
	975*	973	210-8 (20-)	221-4 (18-)	210-7 (11+)	221-6 (9+)
	964*	965	122-6 (21+)	012-8 (10-)	222-2 (6+)	222-4 (5+)
	951*	952	122-6 (29-)	221-6 (15-)	222-6 (6+)	012-8 (5+)
	936*	941	222-6 (19+)	210-5 (9+)	221-2 (7+)	122-2 (6+)
		920	222-6 (28+)	222-2 (13+)	221-6 (12+)	122-6 (4-)
	889*	888	2210-S(13+)	221-5 (11-)	221-6 (7+)	0122-S(7-)
	854*	854	0122-S(21-)	122-5 (21-)	1222-S(10+)	222-5 (9+)
		788	222-6 (35+)	2210-S(17+)	221-6 (8-)	222-6 (6-)
	771*	768	222-5 (21-)	222-5 (20+)	222-6 (9-)	222-6 (8-)
	760*	760	221-5 (24-)	222-5 (12+)	221-6 (11-)	210-5 (11+)
	709*	707	2221-S(25+)	210-5 (15+)	222-6 (15+)	2210-S(10+)
	695*	699	012-5 (44-)	1222-S(13-)	122-5 (13-)	210-5 (5+)
	655*	658	222-4 (18+)	210-5 (15+)	122-6 (14-)	012-8 (12-)
	638*	638	210-8 (20-)	012-8 (17-)	222-4 (15-)	222-4 (14-)
	570*	570	221-4 (31+)	210-8 (25-)	122-4 (18+)	012-8 (13+)
	532*	535	122-4 (42+)	222-4 (25-)	221-4 (13-)	012-8 (12+)
	425	420	222-D (26-)	222-D (21+)	221-D (12+)	122-D (9+)
	335*	331	221-D (39+)	122-D (17-)	222-4 (11+)	222-D (7-)
	263*	261	122-D (41-)	221-D (16-)	222-D (16-)	
		198	222-D (33+)	222-D (16+)	122-D (15-)	221-D (14+)
		170	0122-T(61-)	2210-T(24+)		
		156	2210-T(46+)	0122-T(26+)		
		104	2221-T(35+)	2222-T(16-)	2210-T(14+)	222-D (11-)
		74	1222-T(61+)	2222-T(27+)		
		53	2221-T(43-)	2222-T(32-)	1222-T(10+)	

Calculated frequencies higher than 2000 cm^{-1}
2213 2213 2213 2212 2177 2170 2161 2151 2125 2117
2108 2100 2076 2076

* Weight of the observed frequency is zero.

Reference

[1] IR.R. I. Harada, H. Takeuchi, M. Sakakibara, H. Matsuura, and T. Shimanouchi, Bull. Chem. Soc. Jpn., **50**, 102 (1977).

No. 19

Molecule: 1'2'2'2'2'1'-GTG **$CD_3CD_2CD_2CD_2CD_2CD_3$ (gauche-trans-gauche form)**

Symmetry C_2 **Symmetry number $\sigma = 2$**

Sym. species	Observed frequency cm^{-1}	Calculated frequency cm^{-1}	Assignment (P.E.D. %)			
a	1241*	1238	2222-S(41-)	1222-S(25+)	2221-S(25+)	222-5 (20+)
	1179	1181	2210-S(18-)	0122-S(18-)	221-5 (17-)	122-5 (17+)
	1138*	1135	221-2 (14-)	122-2 (14-)	222-2 (14-)	222-2 (14-)
	1057*	1058	210-2 (23-)	012-2 (23-)	221-5 (8+)	122-5 (8-)
	1057*	1054	122-2 (24-)	221-2 (24-)	012-2 (18+)	210-2 (18+)
	1042*	1046	012-7 (32-)	210-7 (32-)	012-4 (9-)	
	1042*	1043	210-4 (31+)	012-4 (31+)	210-7 (9-)	
	975*	976	122-4 (11+)	221-4 (11-)	012-8 (10-)	210-8 (10-)
	951*	950	221-6 (14-)	122-6 (14-)	222-6 (7-)	222-6 (7-)
	936*	928	222-2 (10-)	222-2 (10-)	210-5 (7+)	012-5 (7+)
	873*	867	2222-S(11-)	222-5 (10+)	222-5 (10-)	2210-S(7-)
	771*	770	222-6 (28+)	222-6 (28+)	0122-S(8+)	2210-S(8+)
	752*	749	2222-S(17+)	012-5 (13-)	210-5 (13-)	221-5 (13+)
	709*	702	122-6 (14-)	221-6 (14-)	012-8 (8-)	210-8 (8-)
	594*	591	222-4 (18+)	222-4 (18-)	012-8 (13+)	210-8 (13+)
		557	222-4 (19-)	222-4 (19+)	221-4 (11-)	122-4 (11+)
	408	408	222-D (16-)	222-D (16-)	122-D (13+)	221-D (13+)
	263*	260	221-D (22+)	122-D (22+)	2222-T(10+)	222-D (9+)
		155	0122-T(42+)	2210-T(42+)		
		79	2221-T(30+)	1222-T(30+)	2222-T(15-)	
		54	2222-T(66-)	1222-T(13-)	2221-T(13-)	
b	1190*	1189	1222-S(23-)	2221-S(23+)	122-5 (18-)	221-5 (18-)
	1152*	1148	122-2 (16-)	221-2 (16+)	0122-S(13-)	2210-S(13+)
	1080*	1078	222-2 (27+)	222-2 (27-)	222-5 (10+)	222-5 (10+)
	1057*	1056	210-2 (40+)	012-2 (40-)		
	1057*	1050	012-4 (18-)	210-4 (18+)	221-2 (10+)	122-2 (10-)
	1042*	1045	210-7 (25-)	012-7 (25+)	210-4 (16-)	012-4 (16+)
		1028	222-5 (14+)	222-5 (14+)	210-7 (10-)	012-7 (10+)
	981*	981	222-4 (19+)	222-4 (19+)	222-6 (8+)	222-6 (8-)
	964*	962	122-6 (17+)	221-6 (17-)	210-8 (12+)	012-8 (12-)
	936*	937	222-6 (17+)	222-6 (17-)	012-5 (6-)	210-5 (6+)
	873*	871	0122-S(9-)	2210-S(9+)	122-5 (8-)	221-5 (8-)
	771*	770	222-5 (19+)	222-5 (19+)	122-6 (14+)	221-6 (14-)
	727*	735	2210-S(12+)	0122-S(12-)	1222-S(11-)	2221-S(11+)
	695*	685	210-5 (16+)	012-5 (16-)	222-4 (13+)	222-4 (13+)
	570*	576	221-4 (26+)	122-4 (26+)	210-8 (22-)	012-8 (22+)
		324	122-D (35+)	221-D (35-)	222-D (9+)	
		229	222-D (24-)	222-D (24+)	0122-T(14-)	2210-T(14+)
		135	2210-T(34+)	0122-T(34-)	222-D (13-)	222-D (13+)
		110	1222-T(37+)	2221-T(37-)		

Calculated frequencies higher than 2000 cm^{-1}

2213 2213 2213 2212 2178 2167 2161 2152 2124 2115
2111 2099 2076 2076

* Weight of the observed frequency is zero.

Reference

[1] IR.R. I. Harada, H. Takeuchi, M. Sakakibara, H. Matsuura, and T. Shimanouchi, Bull. Chem. Soc. Jpn., **50**, 102 (1977).

No. 20

Molecule: 1'2'2'2'2'1'-GTG' $CD_3CD_2CD_2CD_2CD_2CD_3$ (gauche-trans-gauche' form)

Symmetry C_i Symmetry number $\sigma = 1$

Sym. species	Observed frequency cm^{-1}	Calculated frequency cm^{-1}	Assignment (P.E.D. %)			
a_g	1241*	1238	2222-S(40+)	1222-S(25-)	2221-S(25-)	222-5 (20-)
	1179	1183	0122-S(18-)	2210-S(18-)	122-5 (17+)	221-5 (17-)
	1138*	1136	222-2 (14+)	222-2 (14+)	122-2 (13+)	221-2 (13+)
	1057*	1059	012-2 (11-)	210-2 (11-)	222-2 (10+)	222-2 (10+)
	1057*	1055	012-2 (31+)	210-2 (31+)	122-2 (18-)	221-2 (18-)
		1046	012-7 (33-)	210-7 (33+)	012-4 (7-)	
		1043	012-4 (32+)	210-4 (32+)	210-7 (8+)	
	991*	985	222-4 (16-)	222-4 (16-)	122-4 (6+)	221-4 (6+)
	964*	968	012-8 (10-)	210-8 (10+)	122-6 (10+)	221-6 (10-)
	936*	938	222-6 (18+)	222-6 (18-)	221-6 (6+)	122-6 (6-)
	936*	928	222-2 (11+)	222-2 (11+)	012-5 (6-)	210-5 (6-)
	854*	863	2222-S(11+)	222-5 (10-)	222-5 (10+)	2210-S(6+)
	760*	753	2222-S(14-)	2210-S(9+)	0122-S(9+)	210-5 (8+)
	727	726	221-5 (10+)	122-5 (10-)	2222-S(8+)	222-4 (6+)
		681	210-5 (14-)	012-5 (14-)	221-6 (11+)	122-6 (11-)
	570*	573	221-4 (24+)	122-4 (24+)	210-8 (19-)	012-8 (19+)
	408	403	222-D (19+)	222-D (19+)	122-D (12-)	221-D (12-)
		241	221-D (26-)	122-D (26-)	2221-T(7-)	1222-T(7+)
		156	2210-T(41+)	0122-T(41-)		
		112	2221-T(40-)	1222-T(40+)		
a_u	1190*	1187	2221-S(24+)	1222-S(24-)	221-5 (17-)	122-5 (17-)
	1139*	1148	221-2 (16+)	122-2 (16-)	0122-S(14-)	2210-S(14+)
	1070*	1078	222-2 (27+)	222-2 (27-)	222-5 (10-)	222-5 (10-)
	1057*	1056	210-2 (40-)	012-2 (40+)		
	1042*	1049	210-4 (15+)	012-4 (15-)	012-7 (11+)	210-7 (11+)
	1042*	1045	210-7 (22-)	012-7 (22-)	210-4 (20+)	012-4 (20-)
		1028	222-5 (14+)	222-5 (14+)	210-7 (10+)	012-7 (10+)
		965	210-8 (10+)	012-8 (10+)	221-6 (9-)	122-6 (9-)
	959*	949	122-6 (13+)	221-6 (13+)	222-6 (8+)	222-6 (8+)
	872*	876	0122-S(11+)	2210-S(11-)	122-5 (9+)	221-5 (9+)
	773*	778	222-5 (15+)	222-5 (15+)	222-6 (11+)	222-6 (11+)
	760*	757	222-6 (17-)	222-6 (17-)	122-6 (14+)	221-6 (14+)
	719*	718	210-5 (19-)	012-5 (19+)	2221-S(7-)	1222-S(7+)
	595*	595	012-8 (17+)	210-8 (17+)	222-4 (14+)	222-4 (14-)
		554	222-4 (24-)	222-4 (24+)	122-4 (11+)	221-4 (11-)
		345	221-D (35+)	122-D (35-)	2222-T(8-)	
		231	222-D (28-)	222-D (28+)	0122-T(16+)	2210-T(16+)
		134	0122-T(32+)	2210-T(32+)	222-D (16-)	222-D (16+)
		77	2222-T(29-)	1222-T(21+)	2221-T(21+)	
		54	2222-T(53+)	1222-T(20+)	2221-T(20+)	

Calculated frequencies higher than 2000 cm^{-1}

2213 2213 2213 2212 2179 2165 2163 2152 2124 2115
2111 2099 2076 2076

* Weight of the observed frequency is zero.

Reference

[1] IR.R. I. Harada, H. Takeuchi, M. Sakakibara, H. Matsuura, and T. Shimanouchi, Bull. Chem. Soc. Jpn., 50, 102 (1977).

No. 21
Molecule: (2) $(CH_2)_n$
Symmetry[a] D_{2h}

Sym. species	Observed frequency cm^{-1}	Calculated frequency cm^{-1}	Assignment (P.E.D. %)	
a_g	1440(s)	1436	222-2 (100+)	
	1133(s)	1142	222-D (61+)	2222-S(55-)
a_u	1050(s)	1060	222-6 (97+)	
b_{1g}	1382(s)	1377	222-5 (108+)	2222-S(38-)
	1065(s)	1058	2222-S(77+)	
b_{1u}	725(s)	725	222-4 (76+)	2222-T(24+)
b_{2g}	1295(s)	1304	222-6 (100+)	
b_{2u}	1467(s)	1475	222-2 (100+)	
b_{3g}	1174(s)	1168	222-4 (99+)	
b_{3u}	1175(s)	1171	222-5 (100+)	

[a] The point group given is that to which the symmetry of the molecular chain is isomorphous.

Calculated frequencies higher than 2000 cm^{-1}

2914 2896 2878 2862

References

[1] IR. R. G. Snyder, J. Chem. Phys., **47**, 1316 (1967).
[2] R. R. G. Snyder, J. Mol. Spectrosc., **36**, 222 (1970).
[3] R. F. J. Boerio and J. L. Koenig, J. Chem. Phys., **52**, 3425 (1970).

No. 22
Molecule: (2′) $(CD_2)_n$
Symmetry[a] D_{2h}

Sym. species	Observed frequency cm^{-1}	Calculated frequency cm^{-1}	Assignment (P.E.D. %)		
a_g	1146(s)	1139	222-D (47+)	2222-S(42-)	222-2 (33-)
	974(s)	969	222-2 (68+)	222-D (14+)	2222-S(13-)
a_u		750	222-6 (97+)		
b_{1g}	1250(s)	1252	2222-S(90-)	222-5 (65+)	
	830(s)	823	222-5 (50+)	2222-S(25+)	
b_{1u}	526(s)	524	222-4 (76+)	2222-T(24+)	
b_{2g}	916(s)	922	222-6 (100+)		
b_{2u}	1089(s)	1080	222-2 (99+)		
b_{3g}	991(s)	998	222-4 (95+)		
b_{3u}		886	222-5 (100+)		

[a] The point group given is that to which the symmetry of the molecular chain is isomorphous.

Calculated frequencies higher than 2000 cm^{-1}

2187 2143 2140 2091

References

[1] IR. L. C. Leitch, P. E. Gagnon, and A. Cambron, Can. J. Res., **B28**, 256 (1950).
[2] IR. M. Tasumi, T. Shimanouchi, H. Tanaka, and S. Ikeda, J. Polym. Sci., **A2**, 1607 (1964).
[3] R. R. G. Snyder, J. Mol. Spectrosc., **36**, 222 (1970).
[4] R. F. J. Boerio and J. L. Koenig, J. Chem. Phys., 52, 3425 (1970).

No. 23
Molecule: 1321-T $CH_3OCH_2CH_3$ (trans form)
Symmetry C_s Symmetry number $\sigma = 1$

Sym. species	Observed frequency cm^{-1}	Calculated frequency cm^{-1}	Assignment (P.E.D. %)			
a′	1485	1483	321-2 (85-)			
	1472	1468	013-4 (80+)	013-5 (15+)		
	1462	1462	013-2 (102+)			
	1456	1458	210-4 (72+)	210-5 (11+)		
	1392	1389	321-5 (80+)	3210-S(14+)	210-2 (13+)	
	1365	1372	210-2 (81+)	321-5 (12-)		
	1208	1212	013-5 (53+)	1321-S(24-)	013-4 (10-)	
	1120	1122	0132-S(47+)	3210-S(20+)	210-5 (14-)	321-D (10-)
	1094	1095	210-5 (29+)	013-5 (24-)	1321-S(22-)	0132-S(14+)
	1015	1022	3210-S(53+)	0132-S(29-)		
	853	851	1321-S(62-)	210-5 (28-)	321-5 (14+)	0132-S(10-)
	468	466	132-B (38+)	321-D (32+)	3210-S(10+)	
	298	296	321-D (61-)	132-B (51+)		
a″	1456	1455	013-7 (68+)	210-7 (16-)	013-8 (13+)	
	1445	1451	210-7 (63+)	013-7 (18+)	210-8 (12+)	
	1269	1263	321-6 (68+)	321-4 (11+)		
	1169	1164	321-6 (25-)	013-8 (24-)	210-8 (23+)	321-4 (16+)
	1150	1148	013-8 (56+)	210-8 (15+)	321-4 (10+)	
	815	813	321-4 (61+)	210-8 (48-)		
	252	254	3210-T(81+)	0132-T(18-)		
	200	200	0132-T(79+)	3210-T(17+)		
	126	127	1321-T(93+)			

Calculated frequencies higher than 2000 cm^{-1}
2989 2988 2968 2962 2958 2881 2864 2820

References

[1] IR.R. J. P. Perchard, Spectrochim. Acta, **26A**, 707 (1970).
[2] IR. J. P. Perchard, J. Mol. Structure, **6**, 457 (1970).
[3] IR. T. Kitagawa, K. Ohno, H. Sugeta, and T. Miyazawa, Bull. Chem. Soc. Jpn., **45**, 969 (1972).

No. 24
Molecule: 1321-G $CH_3OCH_2CH_3$ (gauche form)
Symmetry C_1 Symmetry number $\sigma = 1$

Sym. species	Observed frequency cm^{-1}	Calculated frequency cm^{-1}	Assignment (P.E.D. %)			
a	1485*	1479	321-2 (86-)	210-4 (10+)		
	1472*	1468	013-4 (77+)	013-5 (14+)		
	1462*	1463	013-2 (85+)			
	1456*	1458	210-4 (59+)	013-2 (16+)	321-2 (10+)	
	1456*	1455	013-7 (56+)	210-7 (24+)	013-8 (11+)	
	1445*	1453	210-7 (53+)	013-7 (27-)	210-8 (10+)	
	1383	1383	321-5 (80+)	210-2 (15+)	3210-S(13+)	
	1365*	1373	210-2 (79+)	321-5 (14-)		
	1304	1296	321-6 (54+)	321-4 (12+)	210-7 (7-)	
	1208*	1207	013-5 (50+)	1321-S(26-)		
	1164	1162	013-8 (32-)	210-8 (19+)	321-6 (15-)	321-4 (13+)
	1150*	1158	013-8 (45+)	321-6 (15-)	210-8 (15+)	321-4 (10+)
	1120*	1116	210-5 (28+)	013-5 (19-)	1321-S(13-)	0132-S(10+)
	1068	1053	3210-S(46-)	0132-S(26-)	1321-S(11+)	
	979	995	0132-S(45+)	3210-S(28-)	210-5 (12-)	
	843	856	1321-S(62-)	210-5 (19-)	321-5 (10+)	
	800	810	321-4 (57+)	210-8 (46-)		
	468*	467	321-D (59+)	132-B (47-)		
	379	376	132-B (38-)	321-D (31-)	3210-T(9-)	
	239	226	3210-T(83-)			
	192*(g)	196	0132-T(87-)			
	126*	125	1321-T(85+)			

Calculated frequencies higher than 2000 cm^{-1}
2989 2988 2969 2962 2959 2881 2864 2820

* Weight of the observed frequency is zero.

References

[1] IR.R. J. P. Perchard, Spectrochim. Acta, **26A**, 707 (1970).
[2] IR. J. P. Perchard, J. Mol. Structure, **6**, 457 (1970).
[3] IR. T. Kitagawa, K. Ohno, H. Sugeta, and T. Miyazawa, Bull. Chem. Soc. Jpn., **45**, 969 (1972).

No. 25
Molecule: 1′321-T $CD_3OCH_2CH_3$ (trans form)
Symmetry C_s Symmetry number σ = 1

Sym. species	Observed frequency cm^{-1}	Calculated frequency cm^{-1}	Assignment (P.E.D. %)			
a′	1482	1482	321-2 (87-)			
	1458	1459	210-4 (75+)	210-5 (11+)		
	1394	1388	321-5 (80+)	210-2 (16+)	3210-S(15+)	
	1370(s)	1372	210-2 (78+)	321-5 (15-)		
	1141	1148	1321-S(45+)	210-5 (31-)		
	1133	1140	0132-S(58+)	013-2 (58+)		
	1092	1090	013-2 (39-)	3210-S(27+)	1321-S(12-)	
	1053	1047	013-4 (90-)			
	993	1000	3210-S(39+)	0132-S(22-)	210-5 (9+)	013-2 (7+)
	957	946	013-5 (48+)	210-5 (18-)	0132-S(12-)	
	809	801	1321-S(49-)	013-5 (31-)	210-5 (14-)	
	447	445	321-D (40+)	132-B (29+)	3210-S(10+)	
	276	278	132-B (57+)	321-D (53-)		
a″	1444	1452	210-7 (79+)	210-8 (15+)		
	1272	1260	321-6 (72+)	321-4 (11+)		
	1159(s)	1159	210-8 (38+)	321-4 (26+)	321-6 (22-)	210-7 (11-)
	1053	1039	013-7 (93+)			
	899	902	013-8 (85+)			
	809	809	321-4 (59-)	210-8 (46+)		
	246	250	3210-T(92+)			
	162	158	0132-T(82+)	1321-T(10-)		
	122	117	1321-T(85+)	0132-T(11+)		

Calculated frequencies higher than 2000 cm^{-1}
2968 2962 2958 2881 2865 2234 2230 2035

References

[1] IR.R. J. P. Perchard, Spectrochim. Acta, **26A**, 707 (1970).
[2] IR. J. P. Perchard, J. Mol. Structure, **6**, 457 (1970).
[3] IR. T. Kitagawa, K. Ohno, H. Sugeta, and T. Miyazawa, Bull. Chem. Soc. Jpn., **45**, 969 (1972).

No. 26
Molecule: 1'321-G $CD_3OCH_2CH_3$ (gauche form)
Symmetry C_1 Symmetry number $\sigma = 1$

Sym. species	Observed frequency cm^{-1}	Calculated frequency cm^{-1}	Assignment (P.E.D. %)			
a	1482*	1479	321-2 (86-)	210-4 (11+)		
	1458*	1459	210-4 (73+)	321-2 (12+)	210-5 (11+)	
	1444*	1453	210-7 (77+)	210-8 (15+)		
	1379	1382	321-5 (79+)	210-2 (17+)	3210-S(13+)	
	1370*(s)	1372	210-2 (77+)	321-5 (17-)		
	1300	1291	321-6 (58+)	321-4 (13+)		
	1159*(s)	1161	210-8 (33+)	321-6 (30-)	321-4 (22+)	
	1159*(s)	1154	1321-S(46-)	210-5 (24+)	0132-S(16+)	
	1133*	1119	013-2 (93+)	0132-S(22+)		
	1072	1065	3210-S(48+)	210-5 (15-)	1321-S(12-)	
	1053*	1048	013-4 (88+)			
	1053*	1039	013-7 (92+)			
	957*	966	0132-S(36+)	210-5 (17-)	3210-S(16-)	013-2 (7-)
	944	945	013-5 (46+)	3210-S(12-)	0132-S(9-)	132-B (7+)
	899*	901	013-8 (87-)			
	809*	810	321-4 (28+)	1321-S(26-)	013-5 (23-)	210-8 (21-)
	796	804	321-4 (31+)	1321-S(25+)	210-8 (24-)	0132-S(12+)
	447*	450	321-D (70+)	132-B (33-)		
	360	358	132-B (45+)	321-D (20+)	3210-T(13+)	
	246*	222	3210-T(82-)	132-B (11+)		
	162*	153	0132-T(69-)	1321-T(21+)		
	122*	109	1321-T(68+)	0132-T(27+)		

Calculated frequencies higher than 2000 cm^{-1}
2969 2962 2959 2881 2864 2234 2230 2035

* Weight of the observed frequency is zero.

References

[1] IR.R. J. P. Perchard, Spectrochim. Acta, **26A**, 707 (1970).
[2] IR. J. P. Perchard, J. Mol. Structure, **6**, 457 (1970).
[3] IR. T. Kitagawa, K. Ohno, H. Sugeta, and T. Miyazawa, Bull. Chem. Soc. Jpn., **45**, 969 (1972).

No. 27
Molecule: 132″1-T $CH_3OCHDCH_3$ (trans form)
Symmetry C_1 Symmetry number $\sigma = 1$

Sym. species	Observed frequency cm^{-1}	Calculated frequency cm^{-1}	Assignment (P.E.D. %)			
a	1463	1468	013-4 (78+)	013-5 (14+)		
	1463	1463	013-2 (70+)	210-4 (22-)		
	1454	1460	210-4 (56+)	013-2 (34+)		
	1454	1454	013-7 (80+)	013-8 (15+)		
	1445	1449	210-7 (74+)	210-8 (13+)		
	1378	1381	210-2 (90+)	3210-S(10+)		
	1343	1342	321-5 (65+)	321-6 (19+)	3210-S(10+)	
	1332	1324	321-2 (73+)			
	1210	1210	013-5 (54+)	1321-S(23-)	013-4 (10-)	
	1163(s)	1163	013-8 (75+)	013-7 (12-)		
	1147	1129	0132-S(36+)	3210-S(21+)	321-6 (9-)	210-8 (9+)
	1111	1116	210-8 (20+)	1321-S(12+)	0132-S(12-)	013-5 (11+)
	1089	1090	210-5 (34+)	210-8 (21+)	321-6 (7-)	210-4 (7-)
	1033	1037	0132-S(36+)	3210-S(36-)	321-6 (13+)	
	922	922	321-6 (33+)	1321-S(19-)	321-5 (12-)	3210-S(10+)
	848	842	1321-S(49-)	210-5 (26-)	321-5 (24+)	
	735	722	321-4 (68+)	210-8 (30-)	321-6 (12-)	
	463	462	132-B (38+)	321-D (33+)	3210-S(10+)	
	295	294	321-D (61-)	132-B (51+)		
	240	251	3210-T(83+)	0132-T(16-)		
	213	200	0132-T(80+)	3210-T(15+)		
		125	1321-T(93+)			

Calculated frequencies higher than 2000 cm^{-1}
2989 2988 2962 2962 2918 2880 2820 2157

References

[1] IR.R. J. P. Perchard, Spectrochim. Acta, **26A**, 707 (1970).
[2] IR. J. P. Perchard, J. Mol. Structure, **6**, 457 (1970).

No. 28
Molecule: 132″1-G $CH_3OCHDCH_3$ (gauche form)[a]
Symmetry C_1 **Symmetry number** $\sigma = 1$

Sym. species	Observed frequency cm^{-1}	Calculated frequency cm^{-1}	Assignment (P.E.D. %)			
a	1463*	1468	013-4 (77+)	013-5 (14+)		
	1463*	1463	013-2 (74+)	210-4 (18-)		
	1454*	1460	210-4 (61+)	013-2 (28+)		
	1454*	1454	013-7 (85+)	013-8 (15+)		
	1445*	1451	210-7 (77+)	210-8 (14+)		
	1378*	1381	210-2 (89+)	3210-S(10+)		
	1343*	1343	321-5 (48+)	321-6 (22+)	321-2 (8-)	
	1332*	1320	321-2 (69+)	321-5 (16+)		
	1210*	1210	013-5 (61+)	1321-S(19-)	013-4 (11-)	
	1163*(s)	1166	013-8 (54+)	013-7 (9-)	1321-S(7+)	0132-S(6-)
	1147*	1156	013-8 (26+)	210-5 (16+)	1321-S(12-)	0132-S(10+)
	1111*	1100	210-8 (38+)	210-7 (8-)	013-5 (8-)	321-4 (8+)
	1059	1059	3210-S(45-)	210-5 (19+)	0132-S(9-)	
	1005	1005	0132-S(56+)	321-6 (20+)	210-5 (12-)	3210-S(12-)
	922*	938	321-6 (24+)	1321-S(22-)	321-5 (12-)	3210-S(8+)
	834	841	1321-S(51-)	321-5 (19+)	210-5 (18-)	0132-S(11-)
	735*	727	321-4 (61+)	210-8 (30-)	321-6 (15-)	
	454	457	321-D (67-)	132-B (37+)		
	368	360	132-B (45+)	321-D (23+)	3210-T(10+)	
	240*	226	3210-T(84+)			
	213*	196	0132-T(88+)			
		123	1321-T(87+)			

[a] The OCH_3 group and the protium of the CHD group are in the trans conformation.

Calculated frequencies higher than 2000 cm^{-1}

2989 2988 2962 2962 2919 2880 2820 2157

* Weight of the observed frequency is zero.

References

[1] IR.R. J. P. Perchard, Spectrochim. Acta, **26A**, 707 (1970).
[2] IR. J. P. Perchard, J. Mol. Structure, **6**, 457 (1970).

No. 29
Molecule: 132″1-G′ $CH_3OCHDCH_3$ (gauche′ form)[a]
Symmetry C_1 Symmetry number $\sigma = 1$

Sym. species	Observed frequency cm^{-1}	Calculated frequency cm^{-1}	Assignment (P.E.D. %)			
a	1463*	1468	013-4 (78+)	013-5 (14+)		
	1463*	1463	013-2 (71+)	210-4 (22-)		
	1463*	1460	210-4 (57+)	013-2 (33+)		
	1454*	1455	013-7 (77+)	013-8 (14+)		
	1445*	1450	210-7 (70+)	210-8 (13+)		
	1378*	1381	210-2 (88+)	3210-S(10+)		
	1343*	1342	321-5 (43+)	321-6 (21+)	321-2 (10-)	
	1332*	1321	321-2 (67+)	321-5 (19+)		
	1210*	1207	013-5 (53-)	1321-S(25+)		
	1163*(s)	1160	013-8 (78+)	013-7 (12-)		
	1133	1140	0132-S(42+)	210-8 (16+)	321-4 (10+)	321-2 (8+)
	1111*	1114	210-5 (25+)	013-5 (15-)	210-8 (12-)	1321-S(9-)
	1089*	1080	321-6 (29+)	210-8 (18-)	210-5 (14-)	3210-S(13-)
	1033*	1041	3210-S(45-)	0132-S(14-)	1321-S(11+)	210-5 (9+)
	848*	869	321-5 (28+)	321-6 (28-)	0132-S(15+)	3210-S(13-)
	848*	853	1321-S(62+)	210-5 (15+)	0132-S(14+)	
	735*	724	321-4 (63+)	210-8 (30-)	321-6 (11-)	
	454	462	321-D (64-)	132-B (42+)		
	368	364	132-B (42-)	321-D (26-)	3210-T(10+)	
	240*	226	3210-T(84+)			
	213*	196	0132-T(88+)			
		123	1321-T(87-)			

[a] The OCH_3 group and the deuterium of the CHD group are in the trans conformation.

Calculated frequencies higher than 2000 cm^{-1}

2989 2988 2962 2962 2918 2880 2820 2159

* Weight of the observed frequency is zero.

References

[1] IR.R. J. P. Perchard, Spectrochim. Acta, **26A**, 707 (1970).
[2] IR. J. P. Perchard, J. Mol. Structure, **6**, 457 (1970).

No. 30
Molecule: 132'1-T $CH_3OCD_2CH_3$ (trans form)
Symmetry C_s Symmetry number $\sigma = 1$

Sym. species	Observed frequency cm^{-1}	Calculated frequency cm^{-1}	Assignment (P.E.D. %)			
a'	1462	1467	013-4 (80+)	013-5 (14+)		
	1462	1462	013-2 (81+)	210-4 (16-)		
	1458	1460	210-4 (64+)	013-2 (24+)		
	1375	1378	210-2 (96+)	3210-S(11+)		
	1223(s)	1222	013-5 (44-)	3210-S(15+)	321-5 (13+)	132-B (10-)
	1203	1195	321-5 (34+)	1321-S(32-)	3210-S(20+)	013-5 (14+)
	1107	1114	210-5 (34-)	321-2 (27+)	013-5 (12+)	
	1096	1092	0132-S(62+)	321-2 (19-)		
	1018	1016	321-2 (48+)	0132-S(13+)	321-5 (10-)	3210-S(10-)
	920	929	1321-S(32-)	3210-S(21+)	321-5 (16-)	0132-S(8-)
	832	824	1321-S(42-)	321-5 (34+)	210-5 (23-)	3210-S(10-)
	452	458	132-B (37+)	321-D (34+)		
	294	292	321-D (60-)	132-B (52+)		
a"	1458	1454	013-7 (86+)	013-8 (16+)		
	1442	1446	210-7 (82+)	210-8 (13+)		
	1154	1164	013-8 (79+)	013-7 (13-)		
	1096	1100	210-8 (56+)	321-4 (16+)	210-7 (14-)	
		906	321-6 (84-)			
		679	321-4 (76-)	210-8 (27+)	321-6 (17+)	
	245	248	3210-T(84+)	0132-T(14-)		
	200	199	0132-T(81+)	3210-T(14+)		
	130	124	1321-T(93+)			

Calculated frequencies higher than 2000 cm^{-1}
2989 2988 2962 2961 2880 2820 2216 2102

References

[1] IR.R. J. P. Perchard, Spectrochim. Acta, **26A**, 707 (1970).
[2] IR. T. Kitagawa, K. Ohno, H. Sugeta, and T. Miyazawa, Bull. Chem. Soc. Jpn., **45**, 969 (1972).

No. 31
Molecule: 132'1-G $CH_3OCD_2CH_3$ (gauche form)
Symmetry C_1 Symmetry number $\sigma = 1$

Sym. species	Observed frequency cm^{-1}	Calculated frequency cm^{-1}	Assignment (P.E.D. %)			
a	1462*	1467	013-4 (80+)	013-5 (14+)		
	1462*	1462	013-2 (79+)	210-4 (16-)		
	1458*	1460	210-4 (64+)	013-2 (25+)		
	1458*	1454	013-7 (86+)	013-8 (16+)		
	1442*	1447	210-7 (82+)	210-8 (13+)		
	1375*	1378	210-2 (96+)	3210-S(11+)		
	1203*	1210	013-5 (61+)	1321-S(18-)	013-4 (11-)	
	1179	1171	013-8 (42+)	321-5 (29-)	3210-S(16-)	
	1154*	1153	013-8 (37-)	321-5 (26-)	3210-S(15-)	
	1133*	1149	0132-S(36+)	210-8 (12-)	1321-S(11-)	321-4 (10-)
	1107*	1108	321-2 (33+)	210-5 (20-)	210-8 (12-)	3210-S(10+)
	1096*	1079	0132-S(30+)	210-8 (30+)	321-2 (15+)	
	1028*	1019	321-2 (43+)	210-5 (18+)	3210-S(17-)	
	937	938	321-6 (31+)	1321-S(24-)	321-5 (9-)	013-5 (8-)
	876	866	321-6 (36+)	321-5 (21+)	0132-S(19+)	3210-S(11-)
	821	829	1321-S(47-)	321-5 (18+)	210-5 (15-)	3210-S(11-)
	689	685	321-4 (67+)	210-8 (26-)	321-6 (20-)	
	452*	454	321-D (69-)	132-B (34+)		
	358	351	132-B (47+)	321-D (21+)	3210-T(10+)	
	233	226	3210-T(84+)			
	200*	196	0132-T(88-)			
	130*	121	1321-T(88+)			

Calculated frequencies higher than 2000 cm^{-1}
2989 2988 2962 2961 2880 2820 2220 2100
* Weight of the observed frequency is zero.

References

[1] IR.R. J. P. Perchard, Spectrochim. Acta, **26A**, 707 (1970).
[2] IR. T. Kitagawa, K. Ohno, H. Sugeta, and T. Miyazawa, Bull. Chem. Soc. Jpn., **45**, 969 (1972).

No. 32
Molecule: 1321'-T **$CH_3OCH_2CD_3$ (trans form)**
Symmetry C_s **Symmetry number σ = 1**

Sym. species	Observed frequency cm^{-1}	Calculated frequency cm^{-1}	Assignment (P.E.D. %)			
a'	1484	1478	321-2 (95+)			
	1461	1467	013-4 (82+)	013-5 (15+)		
	1461	1461	013-2 (101+)			
	1380	1383	321-5 (92+)			
	1201	1206	013-5 (59+)	1321-S(24-)	013-4 (10-)	
	1165	1151	3210-S(55+)	210-2 (47+)		
	1107	1106	0132-S(68+)	1321-S(14-)		
	1043	1048	210-4 (66+)	210-5 (15+)		
	1002	1000	1321-S(36+)	210-4 (24+)	321-D (16-)	210-5 (12-)
	923	925	210-2 (40-)	3210-S(21+)	0132-S(16-)	1321-S(12-)
	731	733	210-5 (57-)	1321-S(27-)		
	441	439	132-B (47+)	321-D (22+)	3210-S(11+)	
	275	275	321-D (68-)	132-B (41+)		
a"	1453	1454	013-7 (86+)	013-8 (16+)		
	1254	1267	321-6 (74+)			
	1144	1155	013-8 (78+)	013-7 (12-)		
	1054	1073	321-4 (45+)	210-8 (24+)	321-6 (17-)	
	1043	1022	210-7 (88+)	321-4 (11-)		
	676	679	210-8 (75+)	321-4 (33-)		
	231	224	0132-T(70-)	3210-T(28+)		
		172	3210-T(70+)	0132-T(26+)		
	125	122	1321-T(92+)			

Calculated frequencies higher than 2000 cm^{-1}
2989 2988 2964 2865 2820 2211 2210 2080

References

[1] IR.R. J. P. Perchard, Spectrochim. Acta, **26A**, 707 (1970).
[2] IR. J. P. Perchard, J. Mol. Structure, **6**, 457 (1970).
[3] IR. T. Kitagawa, K. Ohno, H. Sugeta, and T. Miyazawa, Bull. Chem. Soc. Jpn., **45**, 969 (1972).

No. 33
Molecule: 1321′-G $CH_3OCH_2CD_3$ (gauche form)
Symmetry C_1 Symmetry number $\sigma = 1$

Sym. species	Observed frequency cm^{-1}	Calculated frequency cm^{-1}	Assignment (P.E.D. %)			
a	1484*	1474	321-2 (97+)			
	1461*	1467	013-4 (84+)	013-5 (15+)		
	1461*	1462	013-2 (103+)			
	1453*	1454	013-7 (86+)	013-8 (16+)		
	1380*	1376	321-5 (94+)			
	1293	1300	321-6 (61+)	321-4 (11+)		
	1201*	1204	013-5 (53+)	1321-S(25-)		
	1165*	1159	013-8 (76-)	013-7 (12+)		
	1144*	1143	210-2 (47+)	3210-S(46+)		
	1096*	1098	321-6 (25-)	0132-S(25-)	1321-S(17+)	321-4 (15+)
	1071	1066	321-4 (25+)	210-8 (16+)	1321-S(11-)	210-4 (9+)
	1043*	1041	210-4 (69-)	0132-S(13+)		
		1021	210-7 (77-)	321-4 (10+)		
	949*	953	0132-S(38+)	210-5 (17-)	1321-S(16+)	
	932	926	210-2 (32+)	3210-S(25-)	1321-S(18+)	
	731*	743	210-5 (49-)	1321-S(26-)		
	676	677	210-8 (75-)	321-4 (32+)		
	441*	441	132-B (64+)	321-D (36-)	210-5 (10+)	
	352	357	321-D (45+)	132-B (23+)	1321-T(8-)	
	202	194	0132-T(82+)	321-D (10-)		
		168	3210-T(81-)			
	125*	116	1321-T(82-)			

Calculated frequencies higher than 2000 cm^{-1}
2989 2988 2966 2864 2820 2211 2210 2080

* Weight of the observed frequency is zero.

References

[1] IR.R. J. P. Perchard, Spectrochim. Acta, **26A**, 707 (1970).
[2] IR. J. P. Perchard, J. Mol. Structure, **6**, 457 (1970).
[3] IR. T. Kitagawa, K. Ohno, H. Sugeta, and T. Miyazawa, Bull. Chem. Soc. Jpn., **45**, 969 (1972).

No. 34
Molecule: 1′321′-T $CD_3OCH_2CD_3$ (trans form)
Symmetry C_s Symmetry number σ = 1

Sym. species	Observed frequency cm^{-1}	Calculated frequency cm^{-1}	Assignment (P.E.D. %)			
a′	1481	1477	321-2 (99+)			
	1387	1381	321-5 (95+)			
	1161(g)	1154	3210-S(49-)	210-2 (37-)	1321-S(16+)	
	1142	1137	0132-S(52+)	013-2 (51+)	210-2 (11-)	
	1111	1113	1321-S(44+)	013-2 (33+)	013-5 (10-)	
	1052	1049	013-4 (87+)			
	1042	1038	210-4 (75+)			
	1023	1028	013-2 (18-)	0132-S(17+)	321-D (14-)	132-B (9-)
		914	210-2 (34-)	3210-S(22+)	0132-S(17-)	
	887	888	013-5 (57-)	210-5 (16+)		
	718	717	210-5 (49-)	1321-S(31-)		
	422	417	132-B (38+)	321-D (29+)	3210-S(10+)	
	254	260	321-D (61-)	132-B (48+)		
a″	1253	1264	321-6 (78+)			
	1065(s)	1076	321-4 (46+)	210-8 (24+)	321-6 (20-)	
	1042	1039	013-7 (92+)			
	1023	1023	210-7 (88+)			
	898	898	013-8 (88+)			
	676	678	210-8 (75-)	321-4 (33+)		
	201	202	3210-T(70+)	0132-T(28-)		
	158	147	0132-T(59-)	3210-T(26-)	1321-T(11+)	
		111	1321-T(83+)	0132-T(12+)		

Calculated frequencies higher than 2000 cm^{-1}

2964 2865 2234 2230 2211 2210 2081 2035

References

[1] IR.R. J. P. Perchard, Spectrochim. Acta, **26A**, 707 (1970).
[2] IR. J. P. Perchard, J. Mol. Structure, **6**, 457 (1970).

No. 35
Molecule: 1'321'-G $CD_3OCH_2CD_3$ (gauche form)
Symmetry C_1 Symmetry number σ = 1

Sym. species	Observed frequency cm^{-1}	Calculated frequency cm^{-1}	Assignment (P.E.D. %)			
a	1465	1474	321-2 (101+)			
	1375	1375	321-5 (97+)			
	1288	1296	321-6 (65+)	321-4 (12+)		
	1161*(g)	1156	3210-S(45+)	210-2 (35+)	1321-S(26-)	
	1142*	1127	013-2 (65+)	0132-S(35+)		
	1101	1106	1321-S(38+)	013-2 (28+)	210-2 (12+)	
	1065*(s)	1081	321-4 (41-)	321-6 (27+)	210-8 (20-)	
	1052*	1048	013-4 (87-)			
	1042*	1040	013-7 (90+)			
	1042*	1038	210-4 (77+)			
	1023*	1026	210-7 (88+)			
		954	013-5 (19-)	210-2 (14+)	3210-S(13-)	321-D (11+)
	930	934	0132-S(38+)	013-5 (9-)	210-5 (8-)	210-2 (6-)
	898*	897	013-8 (79-)			
	887*	873	013-5 (38+)	210-2 (12+)	1321-S(12+)	3210-S(10-)
	718*	729	210-5 (44-)	1321-S(31-)		
	676*	676	210-8 (74-)	321-4 (33+)		
	422*	420	132-B (49+)	321-D (48-)	210-5 (11+)	
	341	342	321-D (34+)	132-B (32+)	1321-T(8-)	
	158*	168	3210-T(72-)			
		146	0132-T(71+)	3210-T(14-)		
		103	1321-T(73+)	0132-T(19+)		

Calculated frequencies higher than 2000 cm^{-1}

2966 2864 2234 2230 2211 2210 2080 2035

* Weight of the observed frequency is zero.

References

[1] IR.R. J. P. Perchard, Spectrochim. Acta, **26A**, 707 (1970).
[2] IR. J. P. Perchard, J. Mol. Structure, **6**, 457 (1970).

No. 36
Molecule: 1′32″1′-T $CD_3OCHDCD_3$ (trans form)
Symmetry C_1 Symmetry number $\sigma = 1$

Sym. species	Observed frequency cm^{-1}	Calculated frequency cm^{-1}	Assignment (P.E.D. %)			
a	1348	1337	321-5 (69+)	321-6 (23+)	3210-S(11+)	
	1333	1327	321-2 (88+)			
	1155	1161	3210-S(44+)	210-2 (30+)	1321-S(18-)	
	1135	1137	013-2 (53+)	0132-S(51+)	210-2 (13-)	
	1115	1110	1321-S(42-)	013-2 (31-)	013-5 (10+)	
	1053	1051	013-4 (52+)	210-7 (17+)	013-5 (6+)	
	1053	1046	013-4 (32-)	210-7 (21+)	210-4 (9+)	013-7 (9-)
	1034	1039	013-7 (75+)			
	1034	1038	210-4 (48+)	013-4 (9+)	210-7 (8-)	0132-S(7-)
	1034	1034	210-4 (21-)	321-D (10+)	013-2 (10+)	210-2 (8+)
	990	993	210-7 (35-)	321-4 (22+)	321-5 (6-)	321-2 (6+)
		960	321-6 (25+)	0132-S(16+)	210-2 (14+)	210-8 (11-)
	910	896	013-8 (53+)	013-5 (20+)		
	900	894	013-8 (26-)	013-5 (13+)	3210-S(10+)	210-2 (10-)
	860	853	013-5 (26+)	321-6 (16-)	1321-S(12+)	210-2 (8+)
	716	712	210-5 (47-)	1321-S(28-)	321-5 (10+)	
	625	629	210-8 (58+)	321-4 (46-)		
	416	413	132-B (37+)	321-D (29+)	3210-S(10+)	
	253	258	321-D (60-)	132-B (48+)		
	194	197	3210-T(71+)	0132-T(27-)		
	145	147	0132-T(60+)	3210-T(26+)	1321-T(10-)	
	105	109	1321-T(83+)	0132-T(13+)		

Calculated frequencies higher than 2000 cm^{-1}
2918 2234 2230 2212 2211 2155 2080 2035

References

[1] IR.R. J. P. Perchard, Spectrochim. Acta, **26A**, 707 (1970).
[2] IR. J. P. Perchard, J. Mol. Structure, **6**, 457 (1970).

No. 37
Molecule: 1′32″1′-G $CD_3OCHDCD_3$ (gauche form)[a]
Symmetry C_1 Symmetry number $\sigma = 1$

Sym. species	Observed frequency cm^{-1}	Calculated frequency cm^{-1}	Assignment (P.E.D. %)			
a	1348*	1345	321-5 (42+)	321-6 (22+)	321-2 (19-)	
	1320	1318	321-2 (69+)	321-5 (22+)		
	1155*	1162	3210-S(41+)	210-2 (29+)	1321-S(26-)	0132-S(14+)
	1135*	1127	013-2 (64+)	0132-S(33+)	210-2 (12-)	
	1115*	1104	1321-S(37+)	013-2 (26+)	210-2 (13+)	
	1053*	1070	210-7 (15+)	321-4 (14+)	210-8 (13+)	013-5 (10+)
	1053*	1048	013-4 (87+)			
	1034*	1039	013-7 (89-)			
	1034*	1037	210-4 (78+)			
	1034*	1020	210-7 (72-)			
	990*	979	321-6 (32+)	210-2 (22+)	3210-S(10-)	210-8 (7-)
	930*	931	0132-S(28-)	013-5 (17+)	210-8 (10-)	321-4 (10-)
	906	915	210-5 (23+)	0132-S(19-)	321-6 (15-)	013-8 (8+)
	900*	892	013-8 (65-)	210-2 (7+)		
	839	843	013-5 (37+)	1321-S(12+)	321-6 (10-)	3210-S(9-)
	716*	723	210-5 (42+)	1321-S(28+)	321-5 (9-)	
	625*	630	210-8 (59+)	321-4 (43-)		
	406	411	321-D (56+)	132-B (39-)	210-5 (13-)	
	332	328	132-B (41+)	321-D (26+)	1321-T(8-)	
		167	3210-T(73-)			
	145*	145	0132-T(72+)	3210-T(13-)		
	105*	102	1321-T(75+)	0132-T(18+)		

[a] The OCD_3 group and the protium of the CHD group are in the trans conformation.

Calculated frequencies higher than 2000 cm^{-1}

2919 2234 2230 2212 2211 2155 2080 2035

* Weight of the observed frequency is zero.

References

[1] IR.R. J. P. Perchard, Spectrochim. Acta, **26A**, 707 (1970).

[2] IR. J. P. Perchard, J. Mol. Structure, **6**, 457 (1970).

No. 38
Molecule: 1'32"1'-G' $CD_3OCHDCD_3$ (gauche' form)[a]
Symmetry C_1 **Symmetry number** $\sigma = 1$

Sym. species	Observed frequency cm⁻¹	Calculated frequency cm⁻¹	Assignment (P.E.D. %)			
a	1348*	1342	321-5 (38-)	321-2 (26+)	321-6 (20-)	
	1320	1318	321-2 (61+)	321-5 (28+)		
	1155*	1157	3210-S(50+)	210-2 (38+)	1321-S(21-)	
	1135*	1146	0132-S(62+)	013-2 (47+)		
	1115*	1104	1321-S(37+)	013-2 (28+)	210-2 (12+)	
	1053*	1072	013-2 (27-)	321-5 (13-)	321-4 (10+)	210-7 (9+)
	1053*	1048	013-4 (88-)			
	1034*	1040	013-7 (89+)			
	1034*	1038	210-4 (72+)			
	1034*	1024	210-7 (69-)	210-4 (6+)		
	990*	977	321-6 (21+)	321-4 (19-)	210-2 (18+)	210-8 (14-)
	930*	930	013-5 (22-)	210-5 (18+)	013-8 (14-)	321-6 (11-)
	906	904	013-5 (30+)	0132-S(17-)	210-8 (7+)	210-2 (7+)
	900*	895	013-8 (70+)	210-5 (5+)		
	833	823	0132-S(19-)	321-6 (18+)	1321-S(12-)	013-5 (11-)
	733	726	210-5 (43+)	1321-S(28+)		
	625*	628	210-8 (59+)	321-4 (44-)		
	416*	415	321-D (53+)	132-B (44-)	210-5 (12-)	
	332	331	132-B (37-)	321-D (29-)	1321-T(8-)	
		167	3210-T(73+)			
	145*	146	0132-T(71-)	3210-T(13+)		
	105*	102	1321-T(74+)	0132-T(18+)		

[a] The OCD_3 group and the deuterium of the CHD group are in the trans conformation.

Calculated frequencies higher than 2000 cm⁻¹
2918 2234 2230 2212 2211 2157 2080 2035

* Weight of the observed frequency is zero.

References

[1] IR.R. J. P. Perchard, Spectrochim. Acta, **26A**, 707 (1970).
[2] IR. J. P. Perchard, J. Mol. Structure, **6**, 457 (1970).

No. 39
Molecule: 132'1'-T $CH_3OCD_2CD_3$ (trans form)
Symmetry C_s Symmetry number $\sigma = 1$

Sym. species	Observed frequency cm^{-1}	Calculated frequency cm^{-1}	Assignment (P.E.D. %)			
a'	1463	1467	013-4 (86+)	013-5 (15+)		
	1463	1462	013-2 (106+)			
	1228	1225	013-5 (34+)	3210-S(28-)	321-5 (18-)	
	1187	1197	1321-S(29-)	3210-S(28+)	013-5 (27+)	321-5 (19+)
	1123	1116	0132-S(49-)	210-2 (29+)		
	1091	1093	321-2 (64+)	210-2 (15-)		
	1049	1042	210-4 (71+)	0132-S(10-)		
	1020	1023	321-5 (43-)	0132-S(24+)	210-2 (14+)	321-2 (12+)
	976	970	1321-S(36-)	210-5 (12+)	321-2 (11+)	321-D (10+)
	879	871	3210-S(20+)	210-2 (19-)	1321-S(13-)	321-5 (9-)
	720	717	210-5 (49-)	1321-S(22-)	321-5 (17+)	
	437(s)	433	132-B (46+)	321-D (23+)	3210-S(10+)	
	272	272	321-D (67-)	132-B (42+)		
a"	1452	1454	013-7 (87+)	013-8 (16+)		
	1167	1163	013-8 (81+)	013-7 (13-)		
	1049	1041	210-7 (72+)	210-8 (15+)		
	960	962	321-4 (38+)	210-7 (23-)	210-8 (18+)	
	879	885	321-6 (84-)	210-8 (15+)		
	592	600	321-4 (55-)	210-8 (53+)		
	220	217	0132-T(74+)	3210-T(23-)		
	192*	170	3210-T(75+)	0132-T(22+)		
	122	120	1321-T(92+)			

Calculated frequencies higher than 2000 cm^{-1}
2989 2988 2820 2224 2212 2200 2104 2078

References

[1] IR.R. J. P. Perchard, Spectrochim. Acta, **26A**, 707 (1970).
[2] IR. J. P. Perchard, J. Mol. Structure, **6**, 457 (1970).
[3] IR. T. Kitagawa, K. Ohno, H. Sugeta, and T. Miyazawa, Bull. Chem. Soc. Jpn., **45**, 969 (1972).

No. 40

Molecule: 132'1'-G $CH_3OCD_2CD_3$ (gauche form)

Symmetry C_1 Symmetry number $\sigma = 1$

Sym. species	Observed frequency cm^{-1}	Calculated frequency cm^{-1}	Assignment (P.E.D. %)			
a	1463*	1467	013-4 (85+)	013-5 (15+)		
	1463*	1462	013-2 (105+)			
	1452*	1454	013-7 (87+)	013-8 (16+)		
	1204*	1209	013-5 (63+)	1321-S(18-)	013-4 (11-)	
	1187*	1180	3210-S(57+)	321-5 (31+)	210-2 (20+)	
	1156*	1160	013-8 (72+)	013-7 (11-)		
	1123*	1134	0132-S(57+)	1321-S(14-)		
	1091*	1087	321-2 (71-)	210-2 (12+)		
	1060*	1061	321-5 (38+)	210-2 (30-)	210-4 (17+)	1321-S(14-)
	1049*	1040	210-7 (52+)	210-4 (13+)	210-8 (11+)	
	1020*	1033	210-4 (54+)	210-7 (19-)	321-5 (11-)	
	976*	976	321-4 (22+)	210-7 (20-)	1321-S(15-)	210-8 (7+)
	912	922	0132-S(16-)	210-8 (15-)	210-5 (11+)	321-6 (9+)
	879*	886	321-6 (28-)	3210-S(13-)	210-5 (11+)	210-2 (9+)
	859	851	321-6 (42+)	0132-S(20+)	1321-S(12+)	
	733	727	210-5 (41-)	1321-S(21-)	321-5 (15+)	3210-S(12-)
	592*	604	210-8 (53+)	321-4 (48-)	321-6 (10+)	
	418	424	321-D (49-)	132-B (48+)	210-5 (12+)	
	341	336	132-B (35+)	321-D (33+)	1321-T(8-)	
	204*	194	0132-T(84+)			
	192*	167	3210-T(84+)			
	122*	114	1321-T(85+)			

Calculated frequencies higher than 2000 cm^{-1}

2989 2988 2820 2227 2212 2201 2102 2078

* Weight of the observed frequency is zero.

References

[1] IR.R. J. P. Perchard, Spectrochim. Acta, **26A**, 707 (1970).

[2] IR. J. P. Perchard, J. Mol. Structure, **6**, 457 (1970).

[3] IR. T. Kitagawa, K. Ohno, H. Sugeta, and T. Miyazawa, Bull. Chem. Soc. Jpn., **45**, 969 (1972).

No. 41
Molecule: 12321-TT $CH_3CH_2OCH_2CH_3$ (trans-trans form)
Symmetry C_{2v} Symmetry number $\sigma = 2$

Sym. species	Observed frequency cm^{-1}	Calculated frequency cm^{-1}	Assignment (P.E.D. %)			
a_1	1490	1487	321-2 (44-)	123-2 (44-)		
	1456	1459	210-4 (39+)	012-4 (39+)		
	1414	1408	123-5 (44+)	321-5 (44-)		
	1372	1376	012-2 (46+)	210-2 (46+)		
	1168	1158	012-5 (19+)	210-5 (19+)	2321-S(11-)	1232-S(11-)
	1043	1053	3210-S(30+)	0123-S(30+)	2321-S(10-)	1232-S(10-)
	846	852	1232-S(33-)	2321-S(33-)	210-5 (20-)	012-5 (20-)
	440	439	232-B (36+)	123-D (10+)	321-D (10+)	0123-S(8+)
	208	199	232-B (49+)	123-D (34-)	321-D (34-)	
a_2	1443	1451	012-7 (40+)	210-7 (40+)		
		1237	321-6 (39+)	123-6 (39+)		
	1153	1155	210-8 (20+)	012-8 (20+)	321-4 (14+)	123-4 (14-)
	794	802	321-4 (33-)	123-4 (33+)	210-8 (23+)	012-8 (23+)
	231	242	3210-T(46+)	0123-T(46+)		
	120	119	2321-T(46+)	1232-T(46+)		
b_1	1484	1478	123-2 (42+)	321-2 (42-)		
	1456	1458	012-4 (36+)	210-4 (36-)		
	1383	1379	210-2 (35-)	012-2 (35+)	123-5 (13-)	321-5 (13-)
	1351	1358	321-5 (38+)	123-5 (38+)	012-2 (12+)	210-2 (12-)
	1120	1126	1232-S(40-)	2321-S(40+)	012-5 (10+)	210-5 (10-)
	1077	1078	0123-S(22-)	3210-S(22+)	210-5 (15-)	012-5 (15+)
	935	941	3210-S(19-)	0123-S(19+)	012-5 (13+)	210-5 (13-)
	440	432	321-D (51+)	123-D (51-)		
b_2	1443	1453	210-7 (39+)	012-7 (39-)		
	1279	1280	123-6 (34+)	321-6 (34-)	123-4 (7-)	
	1168	1163	012-8 (18+)	210-8 (18-)	123-4 (13-)	321-4 (13-)
	822	825	123-4 (28-)	321-4 (28-)	012-8 (25-)	210-8 (25+)
	245	258	0123-T(47-)	3210-T(47+)		
	120	117	1232-T(44+)	2321-T(44-)		

Calculated frequencies higher than 2000 cm^{-1}

2968 2968 2962 2962 2958 2958 2881 2881 2865 2864

References

[1] IR.R. H. Wieser, W. G. Laidlaw, P. J. Krueger, and H. Fuhrer, Spectrochim. Acta, **24A**, 1055 (1968).

[2] IR. J. P. Perchard, J. Mol. Structure, **6**, 457 (1970).

[3] IR.R. J. P. Perchard, J. C. Monier, and P. Dizabo, Spectrochim. Acta, **27A**, 447 (1971).

No. 42
Molecule: 12321-TG $CH_3CH_2OCH_2CH_3$ (trans-gauche form)
Symmetry C_1 Symmetry number $\sigma = 1$

Sym. species	Observed frequency cm^{-1}	Calculated frequency cm^{-1}	Assignment (P.E.D. %)			
a	1490*	1483	123-2 (80+)			
	1484*	1479	321-2 (80+)	210-4 (10-)		
	1456*	1459	012-4 (42-)	210-4 (33+)		
	1456*	1458	210-4 (40+)	012-4 (33+)		
	1443*	1454	210-7 (69+)	210-8 (14+)		
	1443*	1452	012-7 (73+)	012-8 (14+)		
	1393	1395	123-5 (66-)	321-5 (16+)	0123-S(10+)	
	1383*	1381	321-5 (57+)	012-2 (18-)	210-2 (12+)	3210-S(10+)
	1372*	1373	210-2 (67+)	012-2 (20+)		
	1372*	1371	012-2 (51+)	321-5 (20+)	210-2 (13-)	
	1297	1288	321-6 (48+)	321-4 (10+)	123-5 (10-)	123-6 (7+)
	1267	1254	123-6 (64-)	123-4 (9+)		
	1168*	1162	210-8 (30+)	321-6 (28-)	321-4 (20+)	
	1168*	1159	012-8 (33+)	123-4 (24-)	123-6 (19-)	012-7 (10-)
	1153*	1145	2321-S(47+)	210-5 (29-)	1232-S(10-)	
	1120*	1118	012-5 (43-)	1232-S(14+)	123-D (11-)	012-4 (10+)
	1074	1068	3210-S(34+)	1232-S(18+)	0123-S(16-)	210-5 (15-)
	1023	1030	0123-S(38-)	3210-S(33-)	2321-S(13+)	
	916	927	210-5 (24+)	2321-S(18+)	1232-S(17-)	3210-S(13+)
	846*	855	1232-S(29-)	2321-S(23-)	012-5 (18-)	210-8 (12-)
	822*	815	123-4 (60+)	012-8 (48+)		
	794*	800	321-4 (49+)	210-8 (35-)	1232-S(15+)	
	503	495	321-D (43-)	232-B (29+)	123-D (16+)	
	376	387	321-D (47+)	123-D (21+)	2321-T(4-)	
	318	310	123-D (46-)	232-B (32+)	3210-T(24+)	
	245*	244	0123-T(90-)			
		209	3210-T(67+)	232-B (20-)		
	120*	120	2321-T(72+)	1232-T(10-)		
		95	1232-T(81-)	2321-T(13-)		

Calculated frequencies higher than 2000 cm^{-1}

2969 2968 2962 2962 2959 2958 2881 2881 2865 2864

* Weight of the observed frequency is zero.

References

[1] IR.R. H. Wieser, W. G. Laidlaw, P. J. Krueger, and H. Fuhrer, Spectrochim. Acta, **24A**, 1055 (1968).

[2] IR. J. P. Perchard, J. Mol. Structure, **6**, 457 (1970).

[3] IR.R. J. P. Perchard, J. C. Monier, and P. Dizabo, Spectrochim. Acta, **27A**, 447 (1971).

No. 43
Molecule: 12321-GG $CH_3CH_2OCH_2CH_3$ (gauche-gauche form)
Symmetry C_2 Symmetry number $\sigma = 2$

Sym. species	Observed frequency cm^{-1}	Calculated frequency cm^{-1}	Assignment (P.E.D. %)			
a		1479	123-2 (42-)	321-2 (42-)		
		1458	210-4 (35+)	012-4 (35+)	321-2 (6+)	
		1455	210-7 (36+)	012-7 (36+)		
		1377	210-2 (37+)	012-2 (37+)	123-5 (10-)	321-5 (10+)
		1356	123-5 (40-)	321-5 (40+)	012-2 (10-)	210-2 (10-)
		1304	123-6 (26+)	321-6 (26+)	123-4 (7-)	321-4 (7+)
		1163	012-8 (17-)	210-8 (17-)	123-6 (17+)	321-6 (17+)
		1094	210-5 (27+)	012-5 (27+)	0123-S(6-)	3210-S(6-)
		1023	3210-S(32-)	0123-S(32-)	2321-S(11+)	1232-S(11+)
		859	1232-S(22+)	2321-S(22+)	012-8 (10+)	210-8 (10+)
		804	123-4 (19-)	321-4 (19+)	2321-S(16+)	1232-S(16+)
		471	232-B (57+)	123-D (26-)	321-D (26-)	
		302	321-D (24+)	123-D (24+)	232-B (21+)	0123-T(10+)
		208	3210-T(37+)	0123-T(37+)	232-B (17-)	
		69	1232-T(47+)	2321-T(47+)		
b		1479	321-2 (45+)	123-2 (45-)		
		1460	012-4 (37+)	210-4 (37-)		
		1452	012-7 (39+)	210-7 (39-)		
		1400	321-5 (45+)	123-5 (45+)		
		1375	012-2 (47-)	210-2 (47+)		
		1273	321-6 (33-)	123-6 (33+)	321-4 (5-)	
		1159	210-8 (13-)	012-8 (13+)	321-6 (13+)	123-6 (13-)
		1146	1232-S(17+)	2321-S(17-)	012-5 (14-)	210-5 (14+)
		1050	0123-S(33-)	3210-S(33+)	1232-S(12+)	2321-S(12-)
		908	1232-S(21-)	2321-S(21+)	012-5 (17-)	210-5 (17+)
		801	321-4 (32-)	123-4 (32-)	210-8 (22+)	012-8 (22-)
		468	321-D (42-)	123-D (42+)		
		244	0123-T(44-)	3210-T(44+)		
		142	2321-T(41+)	1232-T(41-)		

Calculated frequencies higher than 2000 cm^{-1}

2970 2968 2962 2962 2959 2958 2881 2881 2864 2864

No. 44
Molecule: 1′2321′-TT $CD_3CH_2OCH_2CD_3$ (trans-trans form)
Symmetry C_{2v} Symmetry number $\sigma = 2$

Sym. species	Observed frequency cm^{-1}	Calculated frequency cm^{-1}	Assignment (P.E.D. %)			
a_1	1488	1482	123-2 (48+)	321-2 (48+)		
	1411	1405	123-5 (44+)	321-5 (44-)		
	1166	1159	3210-S(28+)	0123-S(28+)	210-2 (23+)	012-2 (23+)
	1078	1081	1232-S(24+)	2321-S(24+)	012-5 (13-)	210-5 (13-)
	1042	1037	210-4 (40+)	012-4 (40+)		
	934	937	210-2 (24+)	012-2 (24+)	1232-S(10+)	2321-S(10+)
	704	714	210-5 (34-)	012-5 (34-)	2321-S(16-)	1232-S(16-)
	410	409	232-B (38+)	0123-S(8+)	3210-S(8+)	123-D (8+)
	169	176	232-B (44+)	321-D (35-)	123-D (35-)	
a_2	1248	1241	321-6 (41+)	123-6 (41+)		
	1050	1066	321-4 (22-)	123-4 (22+)	210-8 (13-)	012-8 (13-)
	1042	1021	210-7 (42+)	012-7 (42+)		
	663	674	210-8 (37-)	012-8 (37-)	321-4 (18+)	123-4 (18-)
		188	3210-T(40+)	0123-T(40+)		
		104	1232-T(41+)	2321-T(41+)		
b_1	1472	1473	321-2 (50+)	123-2 (50-)		
	1359	1356	321-5 (52+)	123-5 (52+)		
	1145	1147	0123-S(26+)	3210-S(26-)	012-2 (21+)	210-2 (21-)
	1116	1112	2321-S(38+)	1232-S(38-)		
	1042	1032	012-4 (41-)	210-4 (41+)		
	934	940	012-2 (12-)	210-2 (12+)	0123-S(11+)	3210-S(11-)
	793	790	012-5 (23+)	210-5 (23-)	012-2 (8-)	210-2 (8+)
	387	383	321-D (46+)	123-D (46-)	210-5 (11-)	012-5 (11+)
b_2	1286	1284	123-6 (37+)	321-6 (37-)		
	1078	1083	123-4 (24+)	321-4 (24+)	123-6 (12+)	321-6 (12-)
	1042	1024	012-7 (45-)	210-7 (45+)		
	680	685	012-8 (38-)	210-8 (38+)	123-4 (15-)	321-4 (15-)
		208	0123-T(43-)	3210-T(43+)		
		104	2321-T(40-)	1232-T(40+)		

Calculated frequencies higher than 2000 cm^{-1}
2965 2964 2866 2864 2212 2211 2210 2210 2081 2080

Reference
[1] IR.R. H. Wieser, W. G. Laidlaw, P. J. Krueger, and H. Fuhrer, Spectrochim. Acta, **24A**, 1055 (1968).

No. 45
Molecule: 1′2321′-TG $CD_3CH_2OCH_2CD_3$ (trans-gauche form)
Symmetry C_1 Symmetry number $\sigma = 1$

Sym. species	Observed frequency cm^{-1}	Calculated frequency cm^{-1}	Assignment (P.E.D. %)			
a	1488*	1478	123-2 (91+)			
	1481	1474	321-2 (93+)			
	1389	1391	123-5 (71-)	321-5 (14+)		
	1367	1373	321-5 (82+)	123-5 (12+)		
	1286*	1289	321-6 (52+)	123-5 (13-)	123-6 (10+)	
	1261	1257	123-6 (67-)	321-6 (9+)		
	1166*	1156	3210-S(28-)	0123-S(26+)	210-2 (22-)	012-2 (18+)
	1145*	1148	012-2 (31-)	0123-S(30-)	3210-S(23-)	210-2 (21-)
	1106	1105	2321-S(40+)	1232-S(22-)	210-2 (11+)	
	1088	1083	321-4 (33+)	321-6 (24-)	210-8 (16+)	2321-S(10-)
	1062	1075	123-4 (46-)	012-8 (24+)	123-6 (20-)	
	1050*	1055	012-4 (42+)	210-4 (15+)	012-5 (13+)	1232-S(10-)
	1042*	1034	210-4 (63+)	012-4 (20-)		
	1042*	1028	210-7 (72+)			
	1042*	1023	012-7 (88+)	123-4 (10+)		
	1001	1002	1232-S(28-)	012-4 (19-)	210-7 (15+)	123-D (12+)
	952	947	012-2 (16+)	210-5 (13-)	210-2 (13-)	3210-S(11+)
	934*	921	012-2 (22-)	210-2 (19-)	3210-S(16+)	0123-S(14+)
	783	775	210-5 (38+)	012-5 (14-)	3210-S(6+)	210-2 (6-)
		724	012-5 (42+)	1232-S(17+)	2321-S(12+)	210-5 (12+)
	680*	680	012-8 (73+)	123-4 (32+)		
	663*	674	210-8 (68+)	321-4 (32-)		
	456	454	232-B (35-)	321-D (32+)	123-D (12-)	210-5 (12-)
	344	354	321-D (49+)	123-D (12+)	210-5 (7-)	2321-T(6-)
		282	123-D (59-)	232-B (30+)	3210-T(13+)	
		189	0123-T(84+)			
		155	3210-T(77+)	232-B (13-)		
		105	2321-T(63+)	1232-T(13-)		
		85	1232-T(76+)	2321-T(15+)		

Calculated frequencies higher than 2000 cm^{-1}
2966 2965 2865 2864 2212 2212 2210 2210 2081 2080
* Weight of the observed frequency is zero.

Reference

[1] IR.R. H. Wieser, W. G. Laidlaw, P. J. Krueger, and H. Fuhrer, Spectrochim. Acta, **24A**, 1055 (1968).

No. 46
Molecule: 12'32'1-TT $CH_3CD_2OCD_2CH_3$ (trans-trans form)
Symmetry C_{2v} Symmetry number $\sigma = 2$

Sym. species	Observed frequency cm^{-1}	Calculated frequency cm^{-1}	Assignment (P.E.D. %)			
a_1	1457	1461	210-4 (42+)	012-4 (42+)		
	1375	1379	210-2 (48+)	012-2 (48+)		
	1210	1227	0123-S(20-)	3210-S(20-)	123-5 (20+)	321-5 (20-)
	1131	1141	012-5 (23-)	210-5 (23-)	1232-S(13+)	2321-S(13+)
	1058	1052	123-2 (40+)	321-2 (40+)		
	940	950	2321-S(17-)	1232-S(17-)	0123-S(17+)	3210-S(17+)
	822	816	2321-S(23-)	1232-S(23-)	321-5 (22+)	123-5 (22-)
	420	420	232-B (34+)	321-D (11+)	123-D (11+)	3210-S(7+)
	186	195	232-B (51+)	321-D (32-)	123-D (32-)	
a_2	1441	1446	012-7 (42+)	210-7 (42+)		
	1095	1098	210-8 (30+)	012-8 (30+)	321-4 (8+)	123-4 (8-)
	883	883	321-6 (44+)	123-6 (44+)		
		664	321-4 (41+)	123-4 (41-)	210-8 (13-)	012-8 (13-)
	235	237	3210-T(48-)	0123-T(48-)		
		105	1232-T(48+)	2321-T(48+)		
b_1	1457	1461	012-4 (43-)	210-4 (43+)		
	1375	1378	012-2 (48+)	210-2 (48-)		
	1186	1183	321-5 (24+)	123-5 (24+)	2321-S(22-)	1232-S(22+)
	1120	1115	321-2 (26+)	123-2 (26-)	3210-S(10+)	0123-S(10-)
	1042	1045	210-5 (18+)	012-5 (18-)	1232-S(15-)	2321-S(15+)
	1010	996	321-2 (16-)	123-2 (16+)	1232-S(11-)	2321-S(11+)
	866	863	123-5 (22+)	321-5 (22+)	0123-S(15+)	3210-S(15-)
	430	424	123-D (51-)	321-D (51+)		
b_2	1441	1447	210-7 (42+)	012-7 (42-)		
	1120	1112	012-8 (26+)	210-8 (26-)	123-4 (10-)	321-4 (10-)
	940	935	123-6 (40+)	321-6 (40-)		
	690	693	123-4 (35-)	321-4 (35-)	012-8 (13-)	210-8 (13+)
		251	0123-T(48-)	3210-T(48+)		
		115	2321-T(45-)	1232-T(45+)		

Calculated frequencies higher than 2000 cm^{-1}
2962 2962 2961 2961 2880 2880 2217 2216 2105 2099

Reference

[1] R.IR. H. Wieser, W. G. Laidlaw, P. J. Krueger, and H. Fuhrer, Spectrochim. Acta, **24A**, 1055 (1968).

No. 47
Molecule: 12'32'1-TG $CH_3CD_2OCD_2CH_3$ (trans-gauche form)
Symmetry C_1 Symmetry number $\sigma = 1$

Sym. species	Observed frequency cm^{-1}	Calculated frequency cm^{-1}	Assignment (P.E.D. %)			
a	1457*	1461	210-4 (47+)	012-4 (37-)		
	1457*	1461	012-4 (47+)	210-4 (37+)		
	1441*	1447	210-7 (76+)	210-8 (12+)		
	1441*	1446	012-7 (76+)	012-8 (12+)		
	1375*	1378	012-2 (90+)	0123-S(11+)		
	1375*	1378	210-2 (90+)	3210-S(10+)		
	1210*	1203	123-5 (44+)	0123-S(38-)		
	1168	1166	321-5 (52+)	3210-S(30+)	2321-S(15-)	210-5 (14+)
	1151	1155	1232-S(34+)	012-5 (17-)	2321-S(8-)	123-2 (8+)
	1120*	1123	321-2 (28+)	210-5 (19-)	3210-S(14+)	2321-S(14+)
	1095*	1106	012-8 (32-)	210-8 (12-)	123-4 (11+)	012-7 (8+)
	1095*	1101	210-8 (25+)	012-8 (21-)	123-2 (9+)	321-4 (7+)
	1058*	1059	321-2 (27+)	012-5 (14+)	123-2 (13+)	1232-S(9+)
	1039	1040	123-2 (46-)	321-2 (15+)	123-5 (8-)	210-8 (5+)
	1018	1012	321-2 (22-)	210-5 (15-)	3210-S(15+)	2321-S(13-)
	957	960	2321-S(19-)	0123-S(19+)	321-6 (19+)	1232-S(6-)
	914	911	123-6 (68+)	0123-S(5-)		
	883*	882	321-6 (30-)	123-5 (27+)	0123-S(11+)	123-6 (10+)
	857	850	321-5 (41+)	3210-S(22-)	210-5 (16-)	2321-S(12-)
	800	803	1232-S(38-)	123-5 (21-)	321-6 (19-)	012-5 (17-)
	681	682	123-4 (48+)	321-4 (24-)	012-8 (17+)	123-6 (12+)
	681	679	321-4 (45-)	123-4 (26-)	210-8 (17+)	
	480	476	321-D (49+)	232-B (22-)	123-D (17-)	
	369	372	321-D (41-)	123-D (33-)		
	289	286	3210-T(34+)	232-B (33+)	123-D (32-)	
	235*	239	0123-T(92-)			
		207	3210-T(59+)	232-B (26-)	123-D (10+)	
		114	2321-T(66+)	1232-T(18-)		
		86	1232-T(74+)	2321-T(22+)		

Calculated frequencies higher than 2000 cm^{-1}
2962 2962 2961 2961 2880 2880 2221 2216 2102 2100
* Weight of the observed frequency is zero.

Reference

[1] IR.R. H. Wieser, W. G. Laidlaw, P. J. Krueger, and H. Fuhrer, Spectrochim. Acta, **24A**, 1055 (1968).

No. 48
Molecule: 1'2'32'1'-TT $CD_3CD_2OCD_2CD_3$ (trans-trans form)
Symmetry C_{2v} Symmetry number $\sigma = 2$

Sym. species	Observed frequency cm^{-1}	Calculated frequency cm^{-1}	Assignment (P.E.D. %)			
a_1	1234	1234	0123-S(27+)	3210-S(27+)	123-5 (17-)	321-5 (17+)
	1127	1118	012-2 (19-)	210-2 (19-)	321-2 (11+)	123-2 (11+)
	1065	1062	123-5 (15-)	321-5 (15+)	123-2 (12-)	321-2 (12-)
	1048	1045	210-4 (20+)	012-4 (20+)	123-2 (19+)	321-2 (19+)
	1022	1018	2321-S(19-)	1232-S(19-)	012-4 (17-)	210-4 (17-)
	877	869	210-2 (12+)	012-2 (12+)	3210-S(11-)	0123-S(11-)
	693	698	210-5 (30-)	012-5 (30-)	2321-S(14-)	1232-S(14-)
	390	392	232-B (37+)	123-D (9+)	321-D (9+)	0123-S(7+)
	166	174	232-B (46+)	321-D (34-)	123-D (34-)	
a_2	1048	1039	210-7 (39+)	012-7 (39+)		
	937	946	321-4 (19-)	123-4 (19+)	210-8 (14-)	012-8 (14-)
	877	873	321-6 (46+)	123-6 (46+)		
	588	589	321-4 (30-)	123-4 (30+)	210-8 (26+)	012-8 (26+)
		179	3210-T(44+)	0123-T(44+)		
		94	2321-T(44+)	1232-T(44+)		
b_1	1191	1188	3210-S(29+)	0123-S(29-)	321-5 (18+)	123-5 (18+)
	1117	1115	1232-S(29-)	2321-S(29+)	123-2 (13-)	321-2 (13+)
	1080	1085	321-2 (23-)	123-2 (23+)	012-2 (19-)	210-2 (19+)
	1022	1036	012-4 (41+)	210-4 (41-)		
	984	984	321-5 (19+)	123-5 (19+)	1232-S(10-)	2321-S(10+)
	903	903	012-5 (17-)	210-5 (17+)	0123-S(8+)	3210-S(8-)
	759	757	012-5 (17+)	210-5 (17-)	0123-S(10+)	3210-S(10-)
	379	376	321-D (46+)	123-D (46-)	210-5 (11-)	012-5 (11+)
b_2	1048	1049	012-7 (28-)	210-7 (28+)	012-8 (9-)	210-8 (9+)
	1005	987	012-7 (19-)	210-7 (19+)	123-4 (16-)	321-4 (16-)
	894	894	123-6 (37+)	321-6 (37-)	012-8 (11-)	210-8 (11+)
	602	611	012-8 (27-)	210-8 (27+)	123-4 (25-)	321-4 (25-)
		198	0123-T(44+)	3210-T(44-)		
		103	1232-T(41-)	2321-T(41+)		

Calculated frequencies higher than 2000 cm^{-1}

2225 2224 2212 2212 2201 2200 2107 2101 2078 2077

References

[1] IR.R. H. Wieser, W. G. Laidlaw, P. J. Krueger, and H. Fuhrer, Spectrochim. Acta, **24A**, 1055 (1968).

[2] IR. J. P. Perchard, J. Mol. Structure, **6**, 457 (1970).

[3] IR.R. J. P. Perchard, J. C. Monier, and P. Dizabo, Spectrochim. Acta, **27A**, 447 (1971).

No. 49

Molecule: 1'2'32'1'-TG $CD_3CD_2OCD_2CD_3$ (trans-gauche form)

Symmetry C_1 Symmetry number $\sigma = 1$

Sym. species	Observed frequency cm^{-1}	Calculated frequency cm^{-1}	Assignment (P.E.D. %)			
a	1207	1211	0123-S(58-)	123-5 (35+)	012-2 (12-)	
	1175	1180	3210-S(65+)	321-5 (32+)	210-2 (24+)	
	1135	1131	1232-S(49-)	2321-S(17+)	123-2 (16-)	
	1117*	1108	012-2 (33+)	2321-S(21-)	321-2 (14-)	123-2 (9-)
	1080*	1085	321-2 (52+)	012-2 (15+)	210-2 (14-)	
	1074	1067	321-5 (29-)	210-2 (25+)	123-2 (14-)	2321-S(13+)
	1065*	1060	123-2 (29+)	210-7 (14+)	210-8 (8+)	321-4 (7+)
	1048*	1044	012-7 (46+)	012-8 (11+)	210-4 (10+)	012-4 (8+)
	1048*	1038	012-4 (62+)	012-7 (11-)		
	1022*	1036	210-4 (47+)	321-2 (8+)	321-5 (8-)	012-7 (8-)
	1022*	1026	210-7 (53-)	210-4 (11+)	123-2 (8+)	
	1005*	1007	123-5 (21-)	2321-S(19-)	210-4 (10-)	210-7 (9-)
	970	965	123-4 (32-)	012-7 (21-)	012-8 (14+)	123-6 (5+)
	937*	937	210-8 (23+)	321-4 (23+)	210-7 (9-)	1232-S(9+)
	903*	902	210-5 (15-)	321-6 (9-)	3210-S(9+)	123-6 (9-)
	880*	884	123-6 (52-)	012-8 (9+)	3210-S(7-)	321-6 (6-)
	880*	879	321-6 (32-)	123-6 (21+)	0123-S(6-)	012-5 (6+)
	859	849	321-6 (28+)	0123-S(13-)	012-2 (12+)	1232-S(12+)
	759*	745	210-5 (32+)	321-5 (16-)	3210-S(11+)	210-2 (8-)
	693*	704	012-5 (40+)	1232-S(18+)	123-5 (14+)	2321-S(10+)
	602*	602	123-4 (47+)	012-8 (46+)		
	588*	599	210-8 (45-)	321-4 (44+)		
	433	436	321-D (39-)	232-B (27+)	123-D (14+)	210-5 (12+)
	334	338	321-D (42+)	123-D (24+)	210-5 (6-)	
	265	261	123-D (46-)	232-B (37+)	3210-T(17+)	
		181	0123-T(89+)			
		154	3210-T(76+)	232-B (14-)		
		102	2321-T(59+)	1232-T(20-)		
		78	1232-T(71-)	2321-T(23-)		

Calculated frequencies higher than 2000 cm^{-1}

2227 2224 2212 2212 2202 2200 2104 2102 2078 2078

* Weight of the observed frequency is zero.

References

[1] IR.R. H. Wieser, W. G. Laidlaw, P. J. Krueger, and H. Fuhrer, Spectrochim. Acta, **24A**, 1055 (1968).

[2] IR. J. P. Perchard, J. Mol. Structure, **6**, 457 (1970).

[3] IR.R. J. P. Perchard, J. C. Monier, and P. Dizabo, Spectrochim. Acta, **27A**, 447 (1971).

No. 50
Molecule: 1232'1'-TT $CH_3CH_2OCD_2CD_3$ (trans-trans form)
Symmetry C_s Symmetry number $\sigma = 1$

Sym. species	Observed frequency cm^{-1}	Calculated frequency cm^{-1}	Assignment (P.E.D. %)			
a'	1482	1482	123-2 (87-)			
	1456	1459	012-4 (75+)	012-5 (11+)		
	1394	1390	123-5 (81+)	0123-S(14-)	012-2 (13-)	
	1382	1372	012-2 (81+)	123-5 (12+)		
	1206	1212	3210-S(53-)	321-5 (33-)	210-2 (11-)	
	1136	1140	012-5 (30+)	1232-S(23-)	210-2 (16+)	3210-S(10+)
	1123	1121	2321-S(45-)	1232-S(24+)	321-2 (23-)	
	1085	1084	321-2 (33-)	210-2 (30+)	0123-S(9+)	
	1062	1051	210-4 (33+)	0123-S(23+)	1232-S(11-)	210-2 (9-)
	1049	1033	210-4 (45+)	321-2 (22+)	321-5 (22-)	
	995	999	2321-S(30-)	0123-S(21+)	321-2 (11+)	210-4 (11-)
	929	940	012-5 (21-)	210-5 (17+)	1232-S(16-)	321-D (10+)
	861	853	1232-S(23-)	3210-S(20+)	210-2 (18-)	012-5 (12-)
	724	727	210-5 (48-)	321-5 (19+)	2321-S(14-)	
	426(s)	423	123-D (43-)	232-B (23-)	0123-S(9-)	
	397(s)	396	321-D (50+)	123-D (20-)	232-B (14+)	210-5 (12-)
	195(s)	185	232-B (47+)	321-D (39-)	123-D (29-)	
a''	1442	1452	012-7 (79+)	012-8 (15+)		
	1273	1261	123-6 (72+)	123-4 (11-)		
	1160	1160	012-8 (37-)	123-4 (26+)	123-6 (22+)	012-7 (11+)
	1049	1042	210-7 (70+)	210-8 (15+)		
	970	965	321-4 (37+)	210-7 (25-)	210-8 (16+)	
		886	321-6 (82+)	210-8 (17-)		
	812	812	123-4 (60+)	012-8 (47+)		
	589	600	321-4 (55+)	210-8 (53-)		
		251	0123-T(92+)			
		188	3210-T(85+)	1232-T(12-)		
		111	2321-T(87-)			
		106	1232-T(81+)	3210-T(11+)		

Calculated frequencies higher than 2000 cm^{-1}

2968 2962 2958 2881 2865 2224 2212 2200 2104 2078

References

[1] IR. J. P. Perchard, J. Mol. Structure, **6**, 457 (1970).
[2] IR.R. J. P. Perchard, J. C. Monier, and P. Dizabo, Spectrochim. Acta, **27A**, 447 (1971).

No. 51

Molecule: 1232′1′-TG $CH_3CH_2OCD_2CD_3$ (trans-gauche form)

Symmetry C_1 Symmetry number σ = 1

Sym. species	Observed frequency cm^{-1}	Calculated frequency cm^{-1}	Assignment (P.E.D. %)			
a	1482*	1482	123-2 (87-)			
	1456*	1459	012-4 (75+)	012-5 (11+)		
	1442*	1452	012-7 (79+)	012-8 (15+)		
	1394*	1389	123-5 (80+)	012-2 (15-)	0123-S(15-)	
	1382*	1372	012-2 (79+)	123-5 (15+)		
	1260	1261	123-6 (71+)	123-4 (11-)		
	1175	1180	3210-S(62+)	321-5 (31+)	210-2 (23+)	
	1160*	1159	012-8 (36-)	123-4 (25+)	123-6 (21+)	012-7 (11+)
	1160*	1151	1232-S(41-)	012-5 (28+)	012-4 (8-)	
	1123*	1116	2321-S(38-)	0123-S(16-)	321-2 (12-)	1232-S(10+)
	1085*	1085	321-2 (60+)	0123-S(12-)	210-2 (11-)	
	1062*	1064	321-5 (37+)	210-2 (32-)	2321-S(14-)	210-4 (11+)
	1049*	1044	210-7 (58+)	210-8 (15+)		
	1049*	1034	210-4 (65+)	321-5 (14-)	321-2 (11+)	
	995*	1001	0123-S(34+)	2321-S(14-)	012-5 (8+)	321-2 (8+)
	982	986	210-7 (30-)	321-4 (24+)	012-5 (9-)	321-6 (6+)
	913	901	321-6 (33-)	210-8 (18+)	210-5 (8-)	1232-S(7+)
		893	321-6 (17+)	210-5 (16-)	3210-S(14+)	210-2 (10-)
	820	822	1232-S(41+)	321-6 (24+)	012-5 (14+)	
	812*	812	123-4 (53+)	012-8 (42+)		
	731	736	210-5 (38+)	321-5 (16-)	3210-S(14+)	2321-S(13+)
	589*	601	210-8 (53-)	321-4 (49+)		
		458	321-D (27+)	232-B (25-)	123-D (24-)	210-5 (11-)
		359	321-D (52+)	123-D (26+)		
		280	232-B (42+)	123-D (36-)	3210-T(14+)	
		241	0123-T(84-)			
		157	3210-T(78-)	232-B (13+)		
		108	2321-T(74+)			
		92	1232-T(82-)	2321-T(12-)		

Calculated frequencies higher than 2000 cm^{-1}

2968 2962 2958 2881 2865 2227 2212 2202 2102 2078

* Weight of the observed frequency is zero.

References

[1] IR. J. P. Perchard, J. Mol. Structure, **6**, 457 (1970).

[2] IR.R. J. P. Perchard, J. C. Monier, and P. Dizabo, Spectrochim. Acta, **27A**, 447 (1971).

No. 52

Molecule: 1232'1'-GT $CH_3CH_2OCD_2CD_3$ (gauche-trans form)

Symmetry C_1 Symmetry number $\sigma = 1$

Sym. species	Observed frequency cm^{-1}	Calculated frequency cm^{-1}	Assignment (P.E.D. %)			
a	1482*	1479	123-2 (86-)	012-4 (11+)		
	1456*	1459	012-4 (73+)	123-2 (12+)	012-5 (11+)	
	1442*	1453	012-7 (77+)	012-8 (15+)		
	1394*	1383	123-5 (80-)	012-2 (16+)	0123-S(13+)	
	1382*	1372	012-2 (78+)	123-5 (16+)		
	1302	1296	123-6 (54+)	123-4 (12-)	012-7 (8-)	
	1206*	1205	3210-S(54-)	321-5 (32-)	210-2 (12-)	2321-S(11+)
	1160*	1160	012-8 (33+)	123-6 (28-)	123-4 (22-)	
	1160*	1143	1232-S(40-)	012-5 (28+)	210-2 (8+)	
	1123*	1098	321-2 (52+)	210-2 (25-)		
	1085*	1074	0123-S(22-)	210-2 (15-)	012-5 (14+)	321-5 (13+)
	1062*	1044	210-4 (27-)	210-7 (24+)	0123-S(14-)	1232-S(7+)
	1049*	1041	210-7 (46+)	210-4 (17+)	0123-S(11+)	
	1049*	1031	321-5 (28-)	210-4 (27+)	0123-S(19-)	321-2 (11+)
	982	987	2321-S(41-)	321-2 (14+)	210-4 (11-)	321-D (7+)
	970*	965	321-4 (37+)	210-7 (24-)	210-8 (16+)	
	929*	923	012-5 (23+)	1232-S(18+)	0123-S(14+)	210-5 (10-)
		886	321-6 (82-)	210-8 (16+)		
	861*	859	1232-S(23-)	3210-S(19+)	210-2 (19-)	012-5 (7-)
	812*	811	123-4 (56+)	012-8 (46+)		
	712	713	210-5 (48-)	2321-S(22-)	321-5 (17+)	
	589*	603	321-4 (53-)	210-8 (52+)	321-6 (10+)	
		475	123-D (53-)	232-B (28+)		
		367	123-D (36+)	321-D (15+)	232-B (13+)	1232-T(5-)
		289	321-D (52-)	0123-T(29+)	232-B (20+)	
		206	0123-T(62-)	232-B (21+)	321-D (12-)	
		183	3210-T(87+)			
		112	1232-T(60+)	2321-T(18-)		
		81	2321-T(74+)	1232-T(20+)		

Calculated frequencies higher than 2000 cm^{-1}

2969 2962 2959 2881 2864 2224 2212 2200 2104 2078

* Weight of the observed frequency is zero.

References

[1] IR. J. P. Perchard, J. Mol. Structure, **6**, 457 (1970).

[2] IR.R. J. P. Perchard, J. C. Monier, and P. Dizabo, Spectrochim. Acta, **27A**, 447 (1971).

No. 53
Molecule: 13221-TT $CH_3OCH_2CH_2CH_3$ (trans-trans form)
Symmetry C_s Symmetry number $\sigma = 1$

Sym. species	Observed frequency cm^{-1}	Calculated frequency cm^{-1}	Assignment (P.E.D. %)			
a′	1486	1488	322-2 (46+)	221-2 (40-)		
	1475	1469	013-4 (33+)	322-2 (29+)	221-2 (14+)	210-4 (13+)
	1469(s)	1467	013-4 (50-)	322-2 (14+)	210-4 (10+)	013-5 (10-)
	1465	1461	013-2 (98+)			
	1439	1453	210-4 (52+)	221-2 (34-)		
	1389	1390	322-5 (77-)	3221-S(12-)	221-5 (11+)	
	1381	1379	210-2 (100+)			
	1309	1307	221-5 (73+)	322-5 (11+)	210-5 (10+)	
	1204	1206	013-5 (57+)	1322-S(22-)	013-4 (10-)	
	1131	1134	0132-S(31-)	3221-S(17-)	210-5 (13+)	322-D (10+)
	1096	1090	0132-S(37+)	1322-S(18-)	013-5 (16-)	210-5 (12+)
	1040	1042	2210-S(65-)	3221-S(28+)		
	958	956	1322-S(47-)	0132-S(30-)	2210-S(18+)	
	902	901	210-5 (45-)	3221-S(19-)	1322-S(13-)	221-5 (10+)
	443	441	132-B (56-)	322-D (12-)	3221-S(12-)	221-D (11+)
	418	414	221-D (39+)	322-D (22+)	1322-S(6+)	2210-S(6+)
	205	203	322-D (50-)	221-D (42+)	132-B (27+)	
a″	1460(s)	1463	210-7 (80+)	210-8 (14+)		
	1454	1454	013-7 (86+)	013-8 (16+)		
	1284	1287	221-6 (36+)	322-6 (31+)	210-7 (6+)	
	1249	1266	322-6 (51+)	221-6 (36-)		
	1174	1176	013-8 (29-)	322-4 (21+)	221-4 (17+)	210-8 (13+)
	1150	1143	013-8 (52-)	322-4 (11-)	221-4 (9-)	
	902	897	210-8 (42+)	322-4 (40-)	221-6 (27+)	
	756	759	221-4 (63+)	210-8 (18-)	322-4 (17-)	3221-T(10+)
	223*(g)	233	2210-T(45+)	0132-T(26+)	3221-T(15-)	
	223*(g)	229	2210-T(47+)	0132-T(41-)	3221-T(11+)	
		154	3221-T(52+)	0132-T(32+)		
		113	1322-T(79+)			

Calculated frequencies higher than 2000 cm^{-1}

2989 2988 2965 2962 2962 2904 2880 2871 2863 2820

Reference

[1] IR.R. T. Shimanouchi, Y. Ogawa, M. Ohta, H. Matsuura, and I. Harada, Bull. Chem. Soc. Jpn., **49**, 2999 (1976).

No. 54

Molecule: 13221-TG $CH_3OCH_2CH_2CH_3$ (trans-gauche form)

Symmetry C_1 Symmetry number $\sigma = 1$

Sym. species	Observed frequency cm^{-1}	Calculated frequency cm^{-1}	Assignment (P.E.D. %)			
a	1486*	1488	322-2 (55+)	221-2 (34+)		
	1475*	1472	322-2 (29-)	210-4 (27+)	221-2 (24+)	
	1469*(s)	1467	013-4 (78+)	013-5 (14+)		
	1465*	1463	210-7 (71+)	210-8 (12+)		
	1460*(s)	1461	013-2 (97+)			
	1454*	1454	013-7 (86+)	013-8 (16+)		
	1439*	1452	210-4 (46+)	221-2 (34-)	322-2 (10+)	
	1389*	1389	322-5 (74+)	210-2 (18+)		
	1376	1378	210-2 (87+)	322-5 (16-)		
	1343	1339	221-5 (79+)			
	1284*	1276	221-6 (50+)	322-6 (16-)	210-8 (7-)	
	1249*	1265	322-6 (61+)	221-6 (15+)		
	1204	1206	013-5 (53+)	1322-S(19-)		
	1163	1165	013-8 (40-)	322-4 (11+)	210-5 (9-)	3221-S(7+)
	1141	1145	013-8 (39-)	3221-S(9-)	322-4 (8-)	0132-S(7-)
	1116	1115	0132-S(41+)	2210-S(14-)	1322-S(11-)	322-4 (7-)
	1096*	1093	210-8 (15+)	221-4 (14+)	210-5 (13-)	013-5 (12-)
	1050	1056	0132-S(34+)	2210-S(28+)	3221-S(25-)	
	933	922	1322-S(39-)	210-5 (28+)	0132-S(12-)	221-5 (11-)
	911	904	322-4 (31+)	210-8 (26+)	221-6 (13+)	2210-S(10-)
	876	876	2210-S(36-)	3221-S(19-)	1322-S(11-)	322-D (6+)
	756*	762	221-4 (55+)	210-8 (23-)	1322-S(12+)	
	505	507	322-D (28-)	221-D (24+)	132-B (16-)	3221-S(9-)
	358	358	132-B (45+)	221-D (41+)		
	312	307	322-D (29+)	3221-T(21-)	132-B (20-)	2210-T(19+)
		219	0132-T(73-)	2210-T(10+)		
	195	199	2210-T(66+)	322-D (18-)		
		145	3221-T(57-)	0132-T(17-)		
		106	1322-T(85-)			

Calculated frequencies higher than 2000 cm^{-1}

2989 2988 2965 2962 2962 2905 2880 2869 2864 2820

* Weight of the observed frequency is zero.

Reference

[1] IR.R. T. Shimanouchi, Y. Ogawa, M. Ohta, H. Matsuura, and I. Harada, Bull. Chem. Soc. Jpn., **49**, 2999 (1976).

No. 55
Molecule: 13221-GT $CH_3OCH_2CH_2CH_3$ (gauche-trans form)
Symmetry C_1 Symmetry number $\sigma = 1$

Sym. species	Observed frequency cm^{-1}	Calculated frequency cm^{-1}	Assignment (P.E.D. %)			
a	1486*	1487	221-2 (45-)	322-2 (41+)		
	1475*	1469	013-4 (42+)	322-2 (23+)	210-4 (9+)	
	1469*(s)	1466	013-4 (43-)	322-2 (23+)	210-4 (15+)	
	1465*	1463	210-7 (80+)	210-8 (14+)		
	1460*(s)	1462	013-2 (92+)			
	1454*	1454	013-7 (84+)	013-8 (15+)		
	1439*	1452	210-4 (45+)	221-2 (35-)		
	1381*	1385	322-5 (70-)	210-2 (15-)	221-5 (11+)	3221-S(10-)
	1376*	1379	210-2 (91+)	322-5 (13-)		
	1305*	1308	221-5 (48+)	322-6 (15-)	322-5 (7+)	210-5 (7+)
	1305*	1307	322-6 (36+)	221-5 (23+)	221-6 (9+)	322-4 (6+)
	1268	1270	221-6 (59-)	322-6 (22+)		
	1204*	1204	013-5 (53+)	1322-S(17-)	013-4 (9-)	
	1174*	1178	322-4 (23+)	221-4 (21+)	210-8 (16+)	0132-S(8-)
	1163*	1159	013-8 (77+)	013-7 (12-)		
	1116*	1113	210-5 (23+)	3221-S(14-)	221-D (10+)	221-5 (9-)
	1062(g)	1067	0132-S(39+)	1322-S(25-)	3221-S(18+)	013-5 (11-)
	1040*	1035	2210-S(76+)	3221-S(16-)		
	942	947	1322-S(37-)	0132-S(32-)	3221-S(11+)	
	902*	894	210-8 (37-)	322-4 (35+)	221-6 (24-)	
	876*	881	210-5 (36+)	3221-S(20+)	1322-S(18+)	
	756*	758	221-4 (62-)	322-4 (18+)	210-8 (17+)	3221-T(11-)
	495	491	132-B (40-)	322-D (35+)		
	375	381	132-B (46+)	221-D (12+)	322-D (7+)	3221-T(6+)
	312*	306	221-D (64-)	322-D (29+)	0132-T(12+)	
		229	2210-T(91+)			
		184	0132-T(82-)	322-D (13+)		
		133	3221-T(74-)			
		115	1322-T(83+)			

Calculated frequencies higher than 2000 cm^{-1}

2990 2988 2966 2962 2962 2904 2880 2871 2862 2820

* Weight of the observed frequency is zero.

Reference

[1] IR.R. T. Shimanouchi, Y. Ogawa, M. Ohta, H. Matsuura, and I. Harada, Bull. Chem. Soc. Jpn., **49**, 2999 (1976).

No. 56

Molecule: 13221-GG $CH_3OCH_2CH_2CH_3$ (gauche-gauche form)

Symmetry C_1 Symmetry number $\sigma = 1$

Sym. species	Observed frequency cm^{-1}	Calculated frequency cm^{-1}	Assignment (P.E.D. %)			
a	1486*	1485	322-2 (47+)	221-2 (41+)		
	1475*	1472	322-2 (38-)	210-4 (23+)	221-2 (19+)	
	1469*(s)	1467	013-4 (80+)	013-5 (14+)		
	1465*	1463	210-7 (57+)	013-2 (23+)	210-8 (10+)	
	1460*(s)	1462	013-2 (78+)	210-7 (15-)		
	1454*	1454	013-7 (75+)	013-8 (14+)		
	1439*	1451	210-4 (40+)	221-2 (30-)	013-7 (11-)	
	1381*	1384	322-5 (59+)	210-2 (38+)		
	1376*	1377	210-2 (67-)	322-5 (33+)		
	1343*	1339	221-5 (79+)			
	1284*	1300	322-6 (60+)	322-4 (9+)	0132-S(7-)	
	1268	1272	221-6 (60+)	210-8 (8-)	210-7 (7+)	
	1204*	1203	013-5 (52+)	1322-S(21-)		
	1163*	1165	013-8 (15+)	322-4 (14-)	221-4 (13+)	210-5 (9+)
	1163*	1157	013-8 (65+)	013-7 (10-)		
	1103	1101	013-5 (18+)	1322-S(15+)	210-5 (15+)	0132-S(8-)
	1077	1076	2210-S(41+)	3221-S(29-)	0132-S(7-)	
	1026	1025	0132-S(52+)	2210-S(9+)	221-6 (8-)	210-8 (8-)
	933*	924	210-5 (32-)	1322-S(30+)	221-5 (15+)	322-4 (12-)
	902*	897	210-8 (24+)	322-4 (24+)	1322-S(16+)	2210-S(13-)
	852	857	2210-S(30+)	3221-S(29+)	1322-S(11+)	210-5 (6+)
	756*	764	221-4 (51+)	210-8 (23-)	1322-S(13+)	
	530(g)	518	322-D (53-)	132-B (22+)	221-D (19+)	
	418*	424	132-B (51+)	221-D (23-)	3221-T(10+)	
	292	285	221-D (39-)	322-D (23-)	132-B (15-)	2210-T(11-)
		231	2210-T(43+)	0132-T(25-)	3221-T(8-)	
		190	0132-T(42-)	2210-T(34-)	322-D (10+)	
		157	3221-T(37-)	0132-T(26+)	1322-T(15+)	
		85	1322-T(66+)	3221-T(25+)		

Calculated frequencies higher than 2000 cm^{-1}

2990 2988 2966 2962 2962 2905 2880 2869 2864 2820

* Weight of the observed frequency is zero.

Reference

[1] IR.R. T. Shimanouchi, Y. Ogawa, M. Ohta, H. Matsuura, and I. Harada, Bull. Chem. Soc. Jpn., **49**, 2999 (1976).

No. 57

Molecule: 123221-TTT $CH_3CH_2OCH_2CH_2CH_3$ (trans-trans-trans form)

Symmetry C_s Symmetry number σ = 1

Sym. species	Observed frequency cm^{-1}	Calculated frequency cm^{-1}	Assignment (P.E.D. %)			
a′	1490	1489	322-2 (45-)	221-2 (30+)	123-2 (14-)	
	1487	1482	123-2 (69-)	221-2 (14-)		
	1473	1468	322-2 (47+)	210-4 (23+)	221-2 (17+)	
	1464	1459	012-4 (74+)	012-5 (11+)	123-2 (10+)	
	1452	1453	210-4 (52+)	221-2 (34-)		
	1415	1408	322-5 (42-)	123-5 (42+)		
	1379	1380	210-2 (90+)			
	1370	1377	012-2 (64+)	210-2 (15+)	0123-S(12+)	322-5 (10-)
	1356	1363	123-5 (41-)	322-5 (28-)	012-2 (20-)	221-5 (11+)
	1304	1305	221-5 (68+)	322-5 (16+)	210-5 (10+)	
	1154	1154	012-5 (21+)	1232-S(19-)	210-5 (8+)	322-D (7+)
	1110	1118	2322-S(39+)	1232-S(38-)		
	1099	1096	012-5 (17-)	0123-S(17+)	3221-S(15-)	2322-S(14+)
	1048	1049	2210-S(41+)	3221-S(26-)	2322-S(15+)	0123-S(13-)
	1017	1019	2210-S(36-)	0123-S(32-)	2322-S(19+)	
	908	908	210-5 (41-)	3221-S(13-)	2322-S(12-)	221-5 (10+)
	883	884	1232-S(39-)	012-5 (24-)	3221-S(14+)	123-5 (10-)
	496	501	123-D (37-)	221-D (23+)	232-B (15-)	322-D (10+)
	410	406	322-D (31-)	232-B (29-)	3221-S(13-)	
	314	310	221-D (48+)	123-D (40+)	2322-S(12+)	
		147	322-D (43-)	232-B (40+)	221-D (20+)	123-D (17-)
a″	1460	1463	210-7 (80+)	210-8 (14+)		
	1443	1452	012-7 (79+)	012-8 (15+)		
	1292	1292	322-6 (36+)	221-6 (20+)	123-6 (13-)	322-4 (5+)
	1275	1271	221-6 (50+)	322-6 (17-)	123-6 (13+)	
	1246	1247	123-6 (45+)	322-6 (32+)		
	1170	1166	322-4 (21-)	221-4 (16-)	123-6 (14-)	210-8 (13-)
	1154	1155	012-8 (27+)	123-4 (18-)	322-4 (11+)	221-4 (9+)
	902	898	210-8 (42-)	322-4 (39+)	221-6 (27-)	
	820	813	123-4 (60+)	012-8 (48+)		
	762	759	221-4 (62+)	322-4 (17-)	210-8 (17-)	3221-T(10+)
	257	255	0123-T(81-)			
	237(s)	229	2210-T(89+)			
	195	196	3221-T(57+)	1232-T(24-)		
		113	2322-T(69+)	1232-T(20+)		
		81	1232-T(50+)	3221-T(23+)	2322-T(16-)	

Calculated frequencies higher than 2000 cm^{-1}

2968 2965 2962 2962 2962 2958 2904 2881 2880 2871
2865 2862

Reference

[1] IR.R. T. Shimanouchi, Y. Ogawa, M. Ohta, H. Matsuura, and I. Harada, Bull. Chem. Soc. Jpn., **49**, 2999 (1976).

No. 58
Molecule: 123221-TTG **$CH_3CH_2OCH_2CH_2CH_3$ (trans-trans-gauche form)**
Symmetry C_1 **Symmetry number $\sigma = 1$**

Sym. species	Observed frequency cm^{-1}	Calculated frequency cm^{-1}	Assignment (P.E.D. %)			
a	1490*	1490	322-2 (46-)	221-2 (24-)	123-2 (19-)	
	1487*	1481	123-2 (63-)	221-2 (15+)		
	1473*	1471	322-2 (34-)	210-4 (27+)	221-2 (20+)	
	1464*	1463	210-7 (74+)	210-8 (13+)		
	1460*	1459	012-4 (74+)	012-5 (11+)	123-2 (10+)	
	1452*	1452	210-4 (31+)	012-7 (27-)	221-2 (22-)	
	1443*	1452	012-7 (52+)	210-4 (16+)	221-2 (12-)	012-8 (10+)
	1408	1407	123-5 (44+)	322-5 (42-)		
	1379*	1380	210-2 (88+)			
	1379*	1377	012-2 (69+)	210-2 (15+)	0123-S(11+)	
	1356*	1360	123-5 (42+)	322-5 (40+)	012-2 (15+)	
	1345	1339	221-5 (79+)			
	1283	1283	322-6 (39+)	123-6 (25-)	221-6 (7-)	
	1275*	1270	221-6 (58+)	210-8 (8-)	210-7 (7+)	
	1252	1242	123-6 (42+)	322-6 (37+)		
	1165	1165	221-4 (11-)	322-4 (11+)	012-8 (8-)	123-6 (8+)
	1154*	1158	012-8 (28-)	123-4 (20+)	123-6 (13+)	012-7 (9+)
	1133	1136	1232-S(23+)	012-5 (22-)	322-4 (12-)	210-5 (10+)
	1118	1126	2322-S(49+)	1232-S(15-)	3221-S(11-)	
	1085	1081	2210-S(33+)	3221-S(14-)	012-5 (11-)	0123-S(7+)
	1062	1071	0123-S(35-)	1232-S(20+)	3221-S(12-)	2210-S(6+)
	985	983	2322-S(29-)	0123-S(22+)	210-5 (11+)	221-5 (6-)
	918	908	322-4 (36+)	210-5 (21+)	210-8 (17+)	221-5 (14-)
	896	889	1232-S(29-)	012-5 (23-)	2322-S(18-)	210-8 (10-)
	883*	877	2210-S(31+)	3221-S(28+)	210-5 (11+)	1232-S(8-)
	820	813	123-4 (60+)	012-8 (47+)		
	762*	765	221-4 (54+)	210-8 (24-)		
	489	495	322-D (37-)	221-D (29+)	123-D (10+)	
	439	436	123-D (44+)	232-B (23+)	0123-S(9+)	
	335	332	221-D (48-)	3221-T(13+)	322-D (11-)	
	257	254	0123-T(66-)	3221-T(10+)		
		245	2210-T(33-)	0123-T(24+)	232-B (17+)	123-D (16-)
		192	2210-T(47+)	3221-T(27+)		
		153	322-D (27+)	1232-T(20-)	232-B (19-)	123-D (11+)
		97	2322-T(83+)			
		89	1232-T(60+)	3221-T(24+)		

Calculated frequencies higher than 2000 cm^{-1}

2968 2965 2962 2962 2962 2958 2905 2881 2880 2869
2865 2864

* Weight of the observed frequency is zero.

Reference

[1] IR.R. T. Shimanouchi, Y. Ogawa, M. Ohta, H. Matsuura, and I. Harada, Bull. Chem. Soc. Jpn., **49**, 2999 (1976).

No. 59
Molecule: 123221-TGT $CH_3CH_2OCH_2CH_2CH_3$ (trans-gauche-trans form)
Symmetry C_1 Symmetry number $\sigma = 1$

Sym. species	Observed frequency cm^{-1}	Calculated frequency cm^{-1}	Assignment (P.E.D. %)			
a	1490*	1487	221-2 (44-)	322-2 (40+)		
	1487*	1482	123-2 (84-)			
	1473*	1467	322-2 (51+)	210-4 (27+)	221-2 (13+)	
	1464*	1463	210-7 (80+)	210-8 (14+)		
	1460*	1459	012-4 (74+)	012-5 (11+)		
	1452*	1453	210-4 (48+)	221-2 (35-)		
	1443*	1452	012-7 (78+)	012-8 (15+)		
	1408*	1395	123-5 (68+)	322-5 (14-)	0123-S(10-)	
	1379*	1383	322-5 (48-)	210-2 (22-)	012-2 (10+)	
	1379*	1378	210-2 (83+)	322-5 (14-)		
	1370*	1372	012-2 (74+)			
	1303*	1307	221-5 (71+)	322-5 (12+)	210-5 (10+)	
	1303*	1300	322-6 (42+)	221-6 (16+)	123-5 (9-)	322-4 (7+)
	1265	1271	221-6 (53+)	322-6 (19-)		
	1252	1254	123-6 (61-)	322-6 (10+)		
	1182	1182	322-4 (24+)	221-4 (23+)	210-8 (18+)	1232-S(6-)
	1154*	1159	012-8 (37-)	123-4 (26+)	123-6 (21+)	012-7 (11+)
	1133*	1125	2322-S(35-)	210-5 (19+)	221-D (10+)	322-D (8+)
	1118*	1114	012-5 (39+)	123-D (10+)	0123-S(10-)	1232-S(9-)
	1099*	1089	1232-S(23-)	3221-S(23-)	2322-S(23+)	0123-S(9+)
	1040	1036	2210-S(68+)	3221-S(21-)		
	1017*	1020	0123-S(41+)	2322-S(35-)	2210-S(13+)	
	918*	912	210-8 (25-)	322-4 (18+)	221-6 (16-)	1232-S(11-)
	896*	892	210-5 (30-)	3221-S(22-)	210-8 (13-)	322-4 (13+)
	844	847	1232-S(48-)	012-5 (21-)	123-5 (10-)	2322-S(10-)
	820*	814	123-4 (60+)	012-8 (48+)		
	753	758	221-4 (62-)	322-4 (18+)	210-8 (17+)	3221-T(11-)
	546	539	322-D (25+)	232-B (24-)	123-D (18-)	221-D (9+)
	363	373	322-D (21+)	123-D (16+)	232-B (11+)	2322-S(5+)
	328	325	221-D (36-)	123-D (30+)	232-B (29-)	322-D (17+)
		292	221-D (33+)	123-D (25+)	232-B (9-)	2322-T(8+)
		239	0123-T(84+)			
		228	2210-T(88-)			
		119	3221-T(59+)	2322-T(20+)		
		102	2322-T(62-)	232-B (10-)		
		84	1232-T(85+)			

Calculated frequencies higher than 2000 cm^{-1}

2968 2966 2962 2962 2962 2958 2904 2881 2880 2871
2865 2862

* Weight of the observed frequency is zero.

Reference

[1] IR.R. T. Shimanouchi, Y. Ogawa, M. Ohta, H. Matsuura, and I. Harada, Bull. Chem. Soc. Jpn., 49, 2999 (1976).

No. 60
Molecule: 123221-TGG $CH_3CH_2OCH_2CH_2CH_3$ (trans-gauche-gauche form)
Symmetry C_1 Symmetry number $\sigma = 1$

Sym. species	Observed frequency cm^{-1}	Calculated frequency cm^{-1}	Assignment (P.E.D. %)			
a	1490*	1485	322-2 (45+)	221-2 (38+)		
	1487*	1482	123-2 (81+)			
	1473*	1471	322-2 (41-)	210-4 (25+)	221-2 (18+)	
	1464*	1463	210-7 (73+)	210-8 (13+)		
	1460*	1459	012-4 (74+)	012-5 (11+)		
	1452*	1452	012-7 (32+)	210-4 (29+)	221-2 (19-)	
	1443*	1451	012-7 (46+)	210-4 (19-)	221-2 (15+)	
	1408*	1396	123-5 (67-)	322-5 (15+)	0123-S(10+)	
	1379*	1383	210-2 (54+)	322-5 (34+)		
	1379*	1377	210-2 (47+)	012-2 (26+)	322-5 (25-)	
	1370*	1371	012-2 (56+)	322-5 (20+)	123-5 (12+)	
	1345*	1339	221-5 (79+)			
	1292*	1292	322-6 (50+)	123-5 (9-)	221-6 (9-)	1232-S(8-)
	1275*	1272	221-6 (54+)	123-6 (10+)	210-8 (7-)	
	1252*	1254	123-6 (59+)	322-6 (8-)	123-4 (8-)	
	1165*	1165	322-4 (16-)	221-4 (12+)	210-5 (12+)	322-6 (8+)
	1154*	1159	012-8 (36-)	123-4 (25+)	123-6 (20+)	012-7 (11+)
	1133*	1137	2322-S(41-)	221-4 (9+)	0123-S(8-)	3221-S(8+)
	1118*	1111	012-5 (36+)	1232-S(19-)	012-4 (8-)	123-D (7+)
	1075	1077	2210-S(42+)	3221-S(22-)	210-8 (5+)	322-D (5+)
	1048*	1049	0123-S(41-)	1232-S(19+)	3221-S(8-)	2210-S(7+)
	985*	978	2322-S(41+)	0123-S(16-)	221-6 (10+)	210-5 (10-)
	918*	915	322-4 (27+)	210-5 (25+)	221-5 (15-)	210-8 (12+)
	873	867	2210-S(29-)	3221-S(19-)	1232-S(17+)	322-4 (12+)
	844	852	1232-S(28-)	012-5 (14-)	3221-S(12-)	210-8 (11-)
	820*	815	123-4 (59+)	012-8 (47+)		
	761*	765	221-4 (48+)	210-8 (22-)	322-4 (10+)	
	546	537	322-D (46+)	232-B (19-)	221-D (14-)	
	439*	434	221-D (26+)	232-B (18-)	123-D (16-)	2322-T(6+)
	335*	338	123-D (50+)	221-D (14+)	322-D (13+)	3221-T(13-)
		270	0123-T(36-)	221-D (25-)	232-B (14-)	
		241	0123-T(39-)	2210-T(30+)	232-B (15+)	
		215	2210-T(46+)	0123-T(19+)	221-D (10-)	322-D (10-)
		154	3221-T(41-)	232-B (15+)	2210-T(14-)	2322-T(10+)
		90	1232-T(53+)	2322-T(39+)		
		72	2322-T(33+)	1232-T(29-)	3221-T(25+)	

Calculated frequencies higher than 2000 cm^{-1}
2968 2967 2962 2962 2962 2958 2905 2881 2880 2869
2865 2864

* Weight of the observed frequency is zero.

Reference

[1] IR.R. T. Shimanouchi, Y. Ogawa, M. Ohta, H. Matsuura, and I. Harada, Bull. Chem. Soc. Jpn., **49**, 2999 (1976).

No. 61

Molecule: 123221-GTG $CH_3CH_2OCH_2CH_2CH_3$ (gauche-trans-gauche form)

Symmetry C_1 Symmetry number σ = 1

Sym. species	Observed frequency cm^{-1}	Calculated frequency cm^{-1}	Assignment (P.E.D. %)			
a	1490*	1488	322-2 (54+)	221-2 (34+)		
	1487*	1479	123-2 (85-)	012-4 (10+)		
	1473*	1472	322-2 (32-)	210-4 (29+)	221-2 (24+)	
	1464*	1463	210-7 (74+)	210-8 (13+)		
	1460*	1459	012-4 (73+)	123-2 (12+)	012-5 (11+)	
	1452*	1454	012-7 (70-)	012-8 (14-)		
	1443*	1452	210-4 (44+)	221-2 (32-)		
	1408*	1395	322-5 (60+)	123-5 (19-)		
	1379*	1380	210-2 (45+)	123-5 (41+)	012-2 (11-)	
	1379*	1377	210-2 (55-)	322-5 (19+)	123-5 (17+)	
	1370*	1373	012-2 (73+)	123-5 (19+)		
	1345*	1340	221-5 (78+)			
	1292*	1291	123-6 (40-)	221-6 (16-)	123-4 (9+)	2322-S(8+)
	1265	1272	221-6 (35+)	322-6 (31-)	210-8 (6-)	
	1252	1255	322-6 (43+)	221-6 (16+)	123-6 (12-)	
	1165	1163	012-8 (24-)	123-6 (24+)	123-4 (16+)	012-7 (7+)
	1154*	1154	322-4 (15-)	012-8 (11-)	210-5 (10+)	3221-S(9-)
	1154*	1146	1232-S(41+)	012-5 (27-)	2322-S(11-)	
	1099*	1102	2322-S(17+)	210-5 (15+)	210-8 (14-)	221-4 (13-)
	1085*	1082	2210-S(29-)	3221-S(23+)	012-5 (12+)	0123-S(10-)
	1048*	1048	0123-S(53-)	1232-S(20+)		
	962	958	2322-S(43-)	012-5 (13+)	210-5 (11+)	0123-S(10+)
	918*	907	322-4 (35-)	210-5 (22-)	210-8 (18-)	221-5 (14+)
	896*	889	1232-S(37+)	012-5 (18+)	2322-S(12+)	0123-S(9+)
	883*	882	2210-S(40-)	3221-S(21-)	210-5 (7-)	322-4 (6+)
	820*	808	123-4 (54+)	012-8 (41+)		
	761*	760	221-4 (52+)	210-8 (21-)	2322-S(12+)	
	518	521	123-D (24-)	322-D (21+)	232-B (17+)	221-D (16-)
	410*	421	123-D (56-)	221-D (25+)		
	335*	343	232-B (38-)	0123-T(17-)	221-D (14-)	123-D (9-)
	314*	312	322-D (27+)	221-D (22+)	3221-T(20-)	2210-T(16+)
		221	0123-T(61-)	2210-T(22-)		
		197	2210-T(56-)	0123-T(15+)		
		159	3221-T(38-)	322-D (19-)	232-B (12+)	1232-T(12+)
		106	1232-T(55+)	3221-T(16+)	2322-T(13-)	
		63	2322-T(73+)	1232-T(15+)		

Calculated frequencies higher than 2000 cm^{-1}

2969 2965 2962 2962 2962 2959 2905 2881 2880 2869
2864 2864

* Weight of the observed frequency is zero.

Reference

[1] IR.R. T. Shimanouchi, Y. Ogawa, M. Ohta, H. Matsuura, and I. Harada, Bull. Chem. Soc. Jpn., **49**, 2999 (1976).

No. 62
Molecule: 132221-TTT $CH_3OCH_2CH_2CH_2CH_3$ (trans-trans-trans form)
Symmetry C_s Symmetry number $\sigma = 1$

Sym. species	Observed frequency cm^{-1}	Calculated frequency cm^{-1}	Assignment (P.E.D. %)			
a′	1484	1488	222-2 (42-)	322-2 (30+)	221-2 (15+)	
	1480	1479	322-2 (46-)	221-2 (35+)	210-4 (10+)	
	1474	1468	013-4 (82+)	013-5 (15+)		
	1467	1462	013-2 (100+)			
	1461	1458	210-4 (38+)	222-2 (36+)	322-2 (13+)	
	1444	1450	221-2 (44+)	210-4 (28-)	222-2 (14+)	
	1395	1390	322-5 (78-)	222-5 (13+)	3222-S(11-)	
	1378	1379	210-2 (105+)			
	1367	1347	221-5 (61+)	222-5 (17-)	2221-S(13-)	322-5 (11-)
	1270	1269	222-5 (65+)	221-5 (19+)		
	1206(s)	1203	013-5 (56+)	1322-S(20-)	013-4 (10-)	
	1130	1135	0132-S(26-)	2221-S(14-)	210-5 (11+)	3222-S(10-)
	1103	1097	0132-S(37+)	1322-S(19-)	013-5 (13-)	210-5 (10+)
	1065	1059	3222-S(33+)	2221-S(29-)	2210-S(20+)	
	1022	1020	2210-S(51-)	3222-S(31+)	0132-S(14-)	
	962	957	1322-S(55-)	210-5 (15-)	0132-S(12-)	322-D (10+)
	897	896	210-5 (33-)	2221-S(30-)	2210-S(11-)	1322-S(10+)
	496	507	132-B (36-)	221-D (25+)	322-D (15-)	222-D (11+)
	387	383	322-D (29+)	222-D (27+)	2221-S(7+)	132-B (6-)
	323	319	221-D (45+)	132-B (37+)	3222-S(10+)	
		147	222-D (49+)	322-D (41-)	221-D (21-)	132-B (13+)
a″	1461	1463	210-7 (81+)	210-8 (14+)		
	1452	1454	013-7 (86+)	013-8 (16+)		
	1304	1307	221-6 (38-)	222-6 (28+)	322-6 (12+)	
	1286	1268	322-6 (70+)	222-6 (12-)		
	1227	1249	222-6 (34+)	221-6 (26+)	210-8 (11-)	
	1171	1175	013-8 (27-)	322-4 (17+)	222-4 (15+)	221-4 (12+)
	1148	1144	013-8 (54+)	322-4 (9+)	013-7 (8-)	
	945(s)	947	210-8 (30+)	322-4 (28-)	221-6 (27+)	222-6 (20+)
	810	803	322-4 (28-)	222-4 (26+)	210-8 (22-)	221-4 (19+)
	747(s)	741	221-4 (48+)	222-4 (33-)	210-8 (11-)	
	247(s)	247	2210-T(50+)	3222-T(24-)	0132-T(21+)	
		217	0132-T(55-)	2210-T(38+)		
		152	1322-T(51+)	2221-T(30-)		
		143	3222-T(48+)	2221-T(20+)	0132-T(17+)	
		78	2221-T(40+)	1322-T(40+)		

Calculated frequencies higher than 2000 cm^{-1}
2989 2988 2964 2962 2962 2909 2900 2880 2874 2867
2862 2820

Reference

[1] IR.R. T. Shimanouchi, Y. Ogawa, M. Ohta, H. Matsuura, and I. Harada, Bull. Chem. Soc. Jpn., **49**, 2999 (1976).

No. 63
Molecule: 132221-TTG $CH_3OCH_2CH_2CH_2CH_3$ (trans-trans-gauche form)
Symmetry C_1 Symmetry number $\sigma = 1$

Sym. species	Observed frequency cm^{-1}	Calculated frequency cm^{-1}	Assignment (P.E.D. %)			
a	1484*	1490	222-2 (45-)	322-2 (34+)	221-2 (15-)	
	1480*	1478	221-2 (46+)	322-2 (27+)	210-4 (17+)	
	1474*	1468	013-4 (68+)	013-5 (12+)		
	1467*	1466	210-7 (24+)	222-2 (16+)	322-2 (16+)	013-4 (14-)
	1461*	1462	013-2 (44-)	210-7 (39+)		
	1461*	1461	013-2 (53+)	210-7 (14+)	322-2 (13-)	
	1452*	1454	013-7 (86+)	013-8 (16+)		
	1444*	1452	210-4 (44+)	221-2 (29-)	222-2 (13+)	
	1395	1391	322-5 (76-)	222-5 (13+)	3222-S(11-)	
	1378*	1379	210-2 (102+)			
	1342	1347	221-5 (70+)	2210-S(8+)		
	1313	1315	222-5 (54+)	221-6 (19+)	322-5 (11+)	
	1270*	1273	322-6 (68+)	222-5 (4-)		
	1260*	1265	221-6 (30+)	222-6 (17+)	222-5 (12-)	322-6 (11-)
	1233*	1249	222-6 (49-)	221-6 (16+)	322-4 (7-)	
	1200*	1205	013-5 (56-)	1322-S(22+)	013-4 (10+)	
	1171*	1167	013-8 (42+)	222-4 (9-)	322-4 (9-)	013-7 (7-)
	1142*	1142	013-8 (37-)	322-4 (9-)	222-4 (8-)	2221-S(6-)
	1120*	1122	0132-S(33-)	3222-S(18-)	210-5 (6-)	322-D (6+)
	1098	1096	0132-S(29+)	013-5 (14-)	1322-S(13-)	222-5 (8-)
	1065*	1077	2210-S(37+)	2221-S(31-)	3222-S(7+)	
	970*	985	3222-S(37+)	210-5 (17-)	0132-S(14-)	221-5 (10+)
	962*	960	2210-S(25-)	1322-S(22-)	322-4 (18+)	222-6 (12-)
	952	950	1322-S(33-)	210-8 (20-)	221-6 (17-)	322-D (8+)
	879	884	2221-S(32+)	2210-S(28+)	210-5 (20+)	
	818*	801	222-4 (30-)	322-4 (23+)	221-4 (19+)	210-8 (15-)
	756*	758	221-4 (41+)	222-4 (23+)	210-8 (19-)	
	460	468	221-D (34+)	222-D (34-)	132-B (18+)	
	449	438	132-B (39-)	322-D (21-)	3222-S(14-)	
	326	333	221-D (38+)	322-D (12+)	3222-T(10+)	222-D (9+)
		245	2210-T(51-)	322-D (22+)	132-B (17-)	
		220	0132-T(80-)			
		177	2210-T(36-)	222-D (23+)	322-D (19-)	2221-T(13-)
		139	1322-T(50+)	222-D (13-)	2221-T(13-)	
		120	3222-T(57+)	2221-T(17+)	0132-T(11+)	
		85	2221-T(40+)	1322-T(36+)		

Calculated frequencies higher than 2000 cm^{-1}

2989 2988 2965 2963 2962 2907 2903 2880 2872 2868
2863 2820

* Weight of the observed frequency is zero.

Reference

[1] IR.R. T. Shimanouchi, Y. Ogawa, M. Ohta, H. Matsuura, and I. Harada, Bull. Chem. Soc. Jpn., **49**, 2999 (1976).

No. 64
Molecule: 132221-TGT $CH_3OCH_2CH_2CH_2CH_3$ (trans-gauche-trans form)
Symmetry C_1 Symmetry number $\sigma = 1$

Sym. species	Observed frequency cm^{-1}	Calculated frequency cm^{-1}	Assignment (P.E.D. %)			
a	1484*	1490	322-2 (35+)	222-2 (33+)	221-2 (18-)	
	1480*	1477	322-2 (47+)	221-2 (30+)	210-4 (14+)	
	1474*	1468	013-4 (82+)	013-5 (15+)		
	1467*	1463	210-7 (81+)	210-8 (14+)		
	1461*	1462	013-2 (99+)			
	1461*	1458	222-2 (47+)	210-4 (23+)	322-2 (16-)	
	1452*	1454	013-7 (85+)	013-8 (16+)		
	1444*	1451	221-2 (44+)	210-4 (39-)		
	1385	1387	322-5 (91+)			
	1378*	1379	210-2 (104+)			
	1367*	1361	221-5 (43-)	222-5 (42+)	2221-S(17+)	
	1304*	1302	221-6 (38+)	222-6 (26-)	221-5 (7-)	
	1286*	1292	222-5 (35+)	221-5 (32+)	221-6 (7+)	
	1260	1266	322-6 (66+)	322-4 (9+)		
	1237	1245	222-6 (33+)	221-6 (20+)	210-8 (11-)	210-7 (7+)
	1200*	1203	013-5 (49+)	1322-S(16-)	013-4 (8-)	
	1162	1161	013-8 (54+)	013-7 (8-)	322-4 (5-)	210-5 (4+)
	1142	1141	013-8 (23-)	322-4 (10-)	222-4 (9+)	3222-S(8-)
	1120	1128	0132-S(27-)	2221-S(19+)	3222-S(9-)	210-5 (7-)
	1112	1104	013-5 (17+)	1322-S(17+)	0132-S(14-)	222-4 (8-)
	1054	1057	0132-S(30-)	3222-S(22+)	2210-S(21+)	2221-S(16-)
	1016	1017	2210-S(57+)	3222-S(26-)		
	970	965	322-4 (33-)	210-5 (27-)	222-5 (12+)	221-5 (11+)
	942	937	1322-S(38-)	210-8 (18-)	221-6 (16-)	222-6 (11-)
	839	839	2221-S(30-)	210-5 (17-)	1322-S(17-)	3222-S(6-)
	829	819	210-8 (21-)	222-4 (18+)	322-4 (17+)	221-4 (13+)
	740	740	221-4 (52+)	222-4 (27-)	210-8 (13-)	
	549	555	322-D (23-)	222-D (17+)	132-B (16-)	221-D (11+)
	352	351	132-B (38+)	222-D (18+)	3222-S(12+)	221-D (11+)
	315	322	322-D (37-)	221-D (30-)	132-B (26+)	
	275	278	221-D (31+)	3222-T(26+)	222-D (21-)	
		225	2210-T(81+)			
		214	0132-T(76-)			
		135	3222-T(51+)	0132-T(15+)	1322-T(10+)	
		95	1322-T(53+)	222-D (16-)	2221-T(10+)	
		87	2221-T(68-)	1322-T(18+)		

Calculated frequencies higher than 2000 cm^{-1}
2989 2988 2965 2962 2962 2909 2901 2880 2873 2866
2864 2820

* Weight of the observed frequency is zero.

Reference

[1] IR.R. T. Shimanouchi, Y. Ogawa, M. Ohta, H. Matsuura, and I. Harada, Bull. Chem. Soc. Jpn., **49**, 2999 (1976).

No. 65
Molecule: 132221-GTT $CH_3OCH_2CH_2CH_2CH_3$ (gauche-trans-trans form)
Symmetry C_1 Symmetry number $\sigma = 1$

Sym. species	Observed frequency cm^{-1}	Calculated frequency cm^{-1}	Assignment (P.E.D. %)			
a	1484*	1488	222-2 (43-)	322-2 (25+)	221-2 (18+)	
	1480*	1477	322-2 (48-)	221-2 (35+)	210-4 (10+)	
	1474*	1467	013-4 (81+)	013-5 (15+)		
	1467*	1463	210-7 (81+)	210-8 (14+)		
	1461*	1462	013-2 (95+)			
	1461*	1457	210-4 (41+)	222-2 (30+)	322-2 (13+)	
	1452*	1454	013-7 (85+)	013-8 (15+)		
	1444*	1449	221-2 (41+)	210-4 (22-)	222-2 (18+)	322-2 (14+)
	1385*	1386	322-5 (76-)	222-5 (15+)	3222-S(10-)	
	1378*	1379	210-2 (104+)			
	1342	1347	221-5 (60+)	222-5 (16-)	322-5 (13-)	2221-S(13-)
	1313	1316	322-6 (32-)	221-6 (21+)	222-6 (19-)	
	1286*	1284	322-6 (37+)	221-6 (25+)	222-6 (15-)	
	1270*	1268	222-5 (64+)	221-5 (19+)		
	1233*	1251	222-6 (39+)	221-6 (22+)	210-8 (9-)	210-7 (6+)
	1200*	1201	013-5 (53+)	1322-S(16-)	013-4 (9-)	
	1171*	1176	222-4 (19+)	322-4 (19+)	221-4 (15+)	210-8 (12+)
	1162*	1159	013-8 (75-)	013-7 (12+)		
	1120*	1120	210-5 (19+)	2221-S(18-)	222-D (9+)	221-D (8+)
	1065*	1069	0132-S(40-)	1322-S(26+)	013-5 (10+)	
	1054*	1055	3222-S(33+)	2221-S(26-)	2210-S(26+)	
	1016*	1014	2210-S(45-)	3222-S(38+)		
	952	952	210-8 (23+)	221-6 (22+)	322-4 (20-)	222-6 (17+)
	924	924	0132-S(33+)	1322-S(32+)	210-5 (9+)	
	897*	903	210-5 (35-)	2221-S(26-)	2210-S(11-)	1322-S(10+)
	810*	802	322-4 (28-)	222-4 (25+)	210-8 (22-)	221-4 (20+)
	740*	741	221-4 (48-)	222-4 (33+)	210-8 (11+)	
	496*	490	322-D (45+)	132-B (40-)	221-D (15-)	
	408	411	221-D (36-)	132-B (16+)	222-D (16-)	322-D (5+)
	352*	368	132-B (29+)	222-D (14+)	322-D (10+)	3222-T(5+)
		234	2210-T(60+)	0132-T(11-)	222-D (10+)	
		231	2210-T(30+)	0132-T(27+)	222-D (18-)	221-D (17+)
		168	0132-T(58+)	222-D (18+)	322-D (14-)	221-D (10-)
		137	2221-T(48+)	1322-T(26-)		
		120	3222-T(70-)	222-4 (7+)		
		85	1322-T(43+)	2221-T(40+)		

Calculated frequencies higher than 2000 cm^{-1}
2990 2988 2966 2962 2962 2909 2900 2880 2874 2867
2862 2820

* Weight of the observed frequency is zero.

Reference

[1] IR.R. T. Shimanouchi, Y. Ogawa, M. Ohta, H. Matsuura, and I. Harada, Bull. Chem. Soc. Jpn., 49, 2999 (1976).

No. 66
Molecule: 132221-GTG $CH_3OCH_2CH_2CH_2CH_3$ (gauche-trans-gauche form)
Symmetry C_1 Symmetry number $\sigma = 1$

Sym. species	Observed frequency cm^{-1}	Calculated frequency cm^{-1}	Assignment (P.E.D. %)			
a	1484*	1490	222-2 (47-)	322-2 (30+)	221-2 (17-)	
	1480*	1477	221-2 (46+)	322-2 (24+)	210-4 (19+)	
	1474*	1468	013-4 (71+)	013-5 (13+)		
	1467*	1465	210-7 (36+)	322-2 (14+)	013-4 (13-)	013-2 (11-)
	1461*	1462	013-2 (60+)	210-7 (30+)		
	1461*	1460	013-2 (30+)	322-2 (22+)	210-4 (17-)	222-2 (14+)
	1452*	1454	013-7 (85+)	013-8 (15+)		
	1444*	1452	210-4 (38+)	221-2 (27-)	222-2 (17+)	
	1385*	1387	322-5 (71-)	222-5 (15+)	210-2 (10+)	3222-S(10-)
	1378*	1379	210-2 (95+)			
	1342	1348	221-5 (68+)	2210-S(8+)		
	1313	1316	222-5 (47+)	221-6 (17+)	322-5 (12+)	
	1304*	1298	322-6 (53-)	322-4 (8-)	222-5 (6+)	221-5 (6-)
	1260*	1265	221-6 (31+)	222-6 (18+)	222-5 (14-)	210-8 (7-)
	1233*	1250	222-6 (46-)	221-6 (16+)	322-6 (6+)	210-8 (6-)
	1200*	1200	013-5 (57+)	1322-S(21-)	013-4 (10-)	
	1171*	1167	222-4 (17-)	322-4 (15-)	210-5 (10+)	2221-S(9-)
	1162*	1158	013-8 (80-)	013-7 (12+)		
	1103*	1106	3222-S(16+)	210-5 (11+)	222-5 (9+)	221-4 (8-)
	1065*	1078	2210-S(34+)	2221-S(30-)	3222-S(10+)	
	1065*	1065	0132-S(42-)	1322-S(22+)	013-5 (8+)	
	970*	974	3222-S(44-)	221-6 (12-)	210-8 (11-)	0132-S(10+)
	970*	965	322-4 (21+)	210-5 (20+)	2210-S(20-)	222-6 (15-)
	924	921	1322-S(37-)	0132-S(32-)	210-8 (12-)	
	879	888	2210-S(31-)	2221-S(29-)	210-5 (19-)	
	818*	799	222-4 (31+)	322-4 (24-)	221-4 (18-)	210-8 (13+)
	756*	754	221-4 (43-)	222-4 (21-)	210-8 (19+)	
	509	505	132-B (29+)	322-D (24-)	221-D (15+)	222-D (11-)
	408	406	132-B (44+)	221-D (35-)	222-D (14+)	
	352*	358	322-D (30+)	221-D (15+)	132-B (14+)	3222-T(11+)
		299	222-D (34+)	2210-T(22+)	221-D (13+)	2221-T(10-)
		206	2210-T(58+)	0132-T(23+)		
		179	0132-T(62-)	2210-T(14+)	322-D (12+)	222-D (11-)
		133	1322-T(42+)	2221-T(33-)		
		107	3222-T(28-)	2221-T(20+)	1322-T(18+)	222-4 (12+)
		79	3222-T(41-)	2221-T(27-)	1322-T(23-)	

Calculated frequencies higher than 2000 cm^{-1}
2990 2988 2966 2963 2962 2907 2903 2880 2872 2868
2862 2820

* Weight of the observed frequency is zero.

Reference

[1] IR.R. T. Shimanouchi, Y. Ogawa, M. Ohta, H. Matsuura, and I. Harada, Bull. Chem. Soc. Jpn., **49**, 2999 (1976).

No. 67

Molecule: 132231-TTT $CH_3OCH_2CH_2OCH_3$ (trans-trans-trans form)

Symmetry C_{2h} Symmetry number $\sigma = 2$

Sym. species	Observed frequency cm^{-1}	Calculated frequency cm^{-1}	Assignment (P.E.D. %)			
a_g	1470*	1472	322-2 (43+)	223-2 (43+)		
	1470*	1467	013-4 (38+)	310-4 (38+)		
	1450*	1461	013-2 (49+)	310-2 (49+)		
	1410*	1406	322-5 (43+)	223-5 (43-)	3223-S(13+)	
	1208*	1210	310-5 (27+)	013-5 (27+)	2231-S(10-)	1322-S(10-)
	1138*	1140	3223-S(29-)	0132-S(17-)	2310-S(17-)	322-D (6+)
	1063	1062	0132-S(25+)	2310-S(25+)	3223-S(12-)	1322-S(10-)
	996	996	1322-S(31+)	2231-S(31+)	3223-S(26-)	
	396	403	322-D (23-)	223-D (23-)	3223-S(9-)	132-B (8+)
		339	231-B (38+)	132-B (38+)	3223-S(13+)	
a_u	1451*	1454	310-7 (43+)	013-7 (43+)		
	1286	1274	322-6 (37+)	223-6 (37+)		
	1160	1153	310-8 (40+)	013-8 (40+)		
	823	823	223-4 (43-)	322-4 (43+)	223-6 (17-)	322-6 (17-)
		233	0132-T(37+)	2310-T(37+)	3223-T(21-)	
		131	3223-T(57+)	2310-T(13+)	0132-T(13+)	
		80	1322-T(37+)	2231-T(37+)	3223-T(16-)	
b_g	1450*	1454	013-7 (43-)	310-7 (43+)		
	1270	1271	223-6 (45+)	322-6 (45-)		
	1155*	1163	013-8 (37-)	310-8 (37+)		
	1092*	1080	322-4 (43+)	223-4 (43+)		
		208	2310-T(49+)	0132-T(49-)		
		153	1322-T(48-)	2231-T(48+)		
b_u	1490*	1491	223-2 (49-)	322-2 (49+)		
	1460*	1468	310-4 (42+)	013-4 (42-)		
	1459*	1461	310-2 (51+)	013-2 (51-)		
	1338*	1349	223-5 (46+)	322-5 (46+)		
	1210*	1203	013-5 (27-)	310-5 (27+)	1322-S(13+)	2231-S(13-)
	1122	1115	2310-S(29-)	0132-S(29+)	2231-S(10+)	1322-S(10-)
	938	929	2231-S(33-)	1322-S(33+)	2310-S(19-)	0132-S(19+)
	513	526	132-B (33-)	231-B (33+)	322-D (14-)	223-D (14+)
		150	223-D (57+)	322-D (57-)	231-B (15-)	132-B (15+)

Calculated frequencies higher than 2000 cm^{-1}

2989 2989 2988 2988 2967 2960 2871 2861 2820 2820

* Weight of the observed frequency is zero.

Reference

[1] IR.R. Y. Ogawa, M. Ohta, M. Sakakibara, H. Matsuura, I. Harada, and T. Shimanouchi, Bull. Chem. Soc. Jpn., **50**, 650 (1977).

No. 68
Molecule: 132231-TTG $CH_3OCH_2CH_2OCH_3$ (trans-trans-gauche form)
Symmetry C_1 Symmetry number σ = 1

Sym. species	Observed frequency cm^{-1}	Calculated frequency cm^{-1}	Assignment (P.E.D. %)			
a	1490*	1489	322-2 (57+)	223-2 (41-)		
	1479*	1469	223-2 (36+)	322-2 (23+)	013-4 (19+)	310-4 (11+)
	1468*	1467	013-4 (45-)	310-4 (38+)		
	1460*	1466	310-4 (36+)	013-4 (19+)	223-2 (18-)	322-2 (12-)
	1459*	1462	310-2 (88+)	013-2 (14+)		
	1459*	1461	013-2 (84+)	310-2 (11-)		
	1451*	1454	310-7 (82+)	310-8 (15+)		
	1451*	1454	013-7 (83+)	013-8 (15+)		
	1393	1402	322-5 (50+)	223-5 (40-)	3223-S(12+)	
	1338	1347	223-5 (52+)	322-5 (39+)		
	1301	1299	223-6 (65+)	223-4 (7-)		
	1270	1272	322-6 (79+)			
	1208*	1205	013-5 (57+)	1322-S(21-)	322-5 (11+)	013-4 (10-)
	1208*	1201	310-5 (57-)	2231-S(21+)	310-4 (10+)	
	1160*	1162	013-8 (65+)	013-7 (10-)		
	1155	1159	310-8 (72+)	310-7 (11-)		
	1131*	1138	0132-S(25-)	3223-S(14-)	013-8 (8+)	322-D (7+)
	1108	1108	322-4 (23+)	223-4 (21+)	2310-S(17+)	0132-S(13+)
	1063*	1074	0132-S(28+)	3223-S(23-)	1322-S(17-)	013-5 (14-)
	1053	1054	2231-S(26-)	2310-S(26+)	322-4 (15-)	223-4 (14-)
	970	970	1322-S(53+)	0132-S(21+)	3223-S(15-)	2310-S(11+)
	923	927	2231-S(48-)	2310-S(35-)		
	822	821	223-4 (42-)	322-4 (42+)	322-6 (17-)	223-6 (17-)
	485	499	223-D (42+)	231-B (31-)	132-B (27-)	
	440	438	132-B (35-)	322-D (21-)	3223-S(12-)	231-B (12+)
	365*	371	231-B (44-)	322-D (9-)	223-D (7-)	3223-T(5-)
		242	2310-T(34-)	322-D (34+)	132-B (21-)	223-D (12-)
		217	0132-T(88-)			
		169	2310-T(61-)	223-D (20+)	322-D (19-)	
		140	1322-T(54+)	2231-T(23-)	223-D (11-)	
		107	3223-T(71+)	2231-T(15+)		
		89	2231-T(38+)	1322-T(37+)		

Calculated frequencies higher than 2000 cm^{-1}
2989 2989 2988 2988 2968 2961 2870 2861 2820 2820

* Weight of the observed frequency is zero.

Reference

[1] IR.R. Y. Ogawa, M. Ohta, M. Sakakibara, H. Matsuura, I. Harada, and T. Shimanouchi, Bull. Chem. Soc. Jpn., **50**, 650 (1977).

No. 69
Molecule: 132231-TGT $CH_3OCH_2CH_2OCH_3$ (trans-gauche-trans form)
Symmetry C_2 Symmetry number $\sigma = 2$

Sym. species	Observed frequency cm^{-1}	Calculated frequency cm^{-1}	Assignment (P.E.D. %)			
a	1490	1488	322-2 (48+)	223-2 (48+)		
	1468	1468	013-4 (42+)	310-4 (42+)		
	1459	1462	310-2 (51+)	013-2 (51+)		
	1451	1454	310-7 (43+)	013-7 (43+)		
	1407	1403	322-5 (43-)	223-5 (43+)	3223-S(13-)	
	1285	1288	322-6 (40+)	223-6 (40+)		
	1208	1203	310-5 (28+)	013-5 (28+)	2231-S(11-)	1322-S(10-)
	1155	1161	013-8 (26+)	310-8 (26+)	3223-S(10-)	2310-S(5-)
	1131	1149	3223-S(18-)	310-8 (12-)	013-8 (12-)	0132-S(10-)
	1078	1074	223-4 (23-)	322-4 (23+)	310-5 (7+)	013-5 (7+)
	1032	1033	3223-S(33-)	0132-S(24+)	2310-S(24+)	
	848	861	1322-S(31+)	2231-S(31+)	223-4 (10+)	322-4 (10-)
	365	363	132-B (25+)	231-B (25+)	3223-S(20+)	223-D (7+)
	295	284	223-D (20+)	322-D (20+)	3223-T(16-)	231-B (15-)
	205(s)	216	0132-T(38-)	2310-T(38-)		
		123	3223-T(57+)	1322-T(11+)	2231-T(11+)	
		98	1322-T(29+)	2231-T(29+)	3223-T(14-)	
b	1479	1472	223-2 (40+)	322-2 (40-)		
	1460	1467	310-4 (34+)	013-4 (34-)	310-5 (7+)	
	1459	1461	013-2 (49+)	310-2 (49-)		
	1451	1454	013-7 (43+)	310-7 (43-)		
	1365	1372	223-5 (48+)	322-5 (48+)		
	1247	1249	223-6 (38+)	322-6 (38-)		
	1208	1204	013-5 (28-)	310-5 (28+)	1322-S(10+)	2231-S(10-)
	1155	1152	310-8 (38+)	013-8 (38-)		
	1092	1096	0132-S(40+)	2310-S(40-)		
	1022	1018	322-4 (18+)	223-4 (18+)	2231-S(18+)	1322-S(18-)
	848	835	2231-S(23+)	1322-S(23-)	322-4 (21-)	223-4 (21-)
	568	568	322-D (23-)	223-D (23+)	132-B (17-)	231-B (17+)
	326	325	322-D (30-)	223-D (30+)	231-B (29-)	132-B (29+)
	205(s)	211	2310-T(48+)	0132-T(48-)		
		95	2231-T(44-)	1322-T(44+)		

Calculated frequencies higher than 2000 cm^{-1}

2989 2989 2988 2988 2966 2962 2867 2862 2820 2820

Reference

[1] IR.R. Y. Ogawa, M. Ohta, M. Sakakibara, H. Matsuura, I. Harada, and T. Shimanouchi, Bull. Chem. Soc. Jpn., **50**, 650 (1977).

No. 70
Molecule: 132231-TGG $CH_3OCH_2CH_2OCH_3$ (trans-gauche-gauche form)
Symmetry C_1 Symmetry number $\sigma = 1$

Sym. species	Observed frequency cm^{-1}	Calculated frequency cm^{-1}	Assignment (P.E.D. %)			
a	1490*	1485	322-2 (60+)	223-2 (38+)		
	1479*	1471	223-2 (50+)	322-2 (28-)		
	1468*	1468	013-4 (50+)	310-4 (32+)		
	1460*	1467	310-4 (48+)	013-4 (25-)		
	1459*	1462	310-2 (77+)	013-2 (27-)		
	1459*	1461	013-2 (74+)	310-2 (23+)		
	1451*	1454	310-7 (49+)	013-7 (37-)		
	1451*	1454	013-7 (49+)	310-7 (36+)		
	1393*	1399	322-5 (52+)	223-5 (36-)	3223-S(12+)	
	1372	1370	223-5 (58+)	322-5 (39+)		
	1301	1302	223-6 (58+)	322-6 (14+)		
	1256	1263	322-6 (65-)	223-6 (10+)		
	1208*	1209	013-5 (38-)	310-5 (21+)	1322-S(14+)	
	1195	1201	310-5 (33+)	013-5 (19+)	2231-S(15-)	1322-S(8-)
	1160	1161	013-8 (41-)	310-8 (29-)	013-7 (6+)	
	1155*	1156	310-8 (50+)	013-8 (29-)		
	1138	1131	0132-S(34+)	3223-S(21+)	1322-S(9-)	322-D (5-)
	1108	1108	2310-S(21-)	322-4 (17+)	2231-S(13+)	223-4 (9-)
	1063	1062	0132-S(32-)	3223-S(26+)	2231-S(13-)	
	1022	1018	223-4 (23+)	1322-S(22-)	0132-S(18-)	3223-S(12+)
	985	985	2310-S(51+)	322-4 (31+)		
	868	861	2231-S(41+)	1322-S(23+)	322-4 (9-)	
	848*	833	1322-S(30-)	223-4 (27-)	2231-S(17+)	322-4 (14-)
	540	542	223-D (49-)	322-D (26+)	132-B (14+)	231-B (11+)
	440	431	231-B (59+)	322-D (8-)	3223-S(7-)	
	352	354	132-B (47-)	223-D (25-)		
		266	322-D (42+)	132-B (18-)	231-B (13+)	223-D (10+)
		221	0132-T(62-)	2310-T(18+)	3223-T(10+)	
		198	2310-T(56-)	0132-T(22-)		
		141	2231-T(33-)	3223-T(22+)	2310-T(19-)	
		109	1322-T(62+)	3223-T(24+)		
		68	2231-T(45-)	3223-T(28-)	1322-T(16+)	

Calculated frequencies higher than 2000 cm^{-1}

2990 2989 2988 2988 2967 2963 2867 2862 2820 2820

* Weight of the observed frequency is zero.

Reference

[1] IR.R. Y. Ogawa, M. Ohta, M. Sakakibara, H. Matsuura, I. Harada, and T. Shimanouchi, Bull. Chem. Soc. Jpn., **50**, 650 (1977).

No. 71
Molecule: (322) $(OCH_2CH_2)_n$
Symmetry[a] D_7

Sym. species	Observed frequency cm^{-1}	Calculated frequency cm^{-1}	Assignment (P.E.D. %)			
a_1	1484(s)	1492	223-2 (93+)			
	1398(s)	1424	223-5 (86+)	3223-S(13-)		
	1282(s)	1278	223-6 (90+)			
	1126(s)	1135	3223-S(39-)	223-4 (19+)	223-D (12+)	232-B (9+)
	1064(s)	1067	2232-S(48-)	223-4 (35+)	3223-S(23+)	
	861(s)	851	2232-S(62+)	223-4 (38+)	223-5 (22+)	
	279(s)	273	223-D (37+)	3223-T(21-)	2232-T(18+)	3223-S(12+)
	231(s)	232	232-B (66+)	3223-S(14+)	2232-T(11-)	
a_2	1460(s)	1470	223-2 (99+)			
	1345(s)	1349	223-5 (101+)			
	1244(s)	1260	223-6 (75+)	223-4 (11-)		
	1102(s)	1105	2232-S(92+)	223-4 (14+)		
	963(s)	969	223-4 (58+)	223-6 (21+)	223-D (12-)	2232-S(11-)
	529(s)	523	223-D (97+)	223-4 (11+)	223-5 (10-)	
	107(s)	111	2232-T(90+)			
e_1	1470(s)	1486	223-2 (96+)			
	1453(s)	1473	223-2 (99+)			
	1415(s)	1410	223-5 (89+)			
	1364(s)	1361	223-5 (96+)			
	1282(s)	1297	223-6 (45+)	223-6 (36+)		
	1235(s)	1228	223-6 (45+)	223-6 (40-)		
	1143(s)	1140	2232-S(41-)	3223-S(28+)	223-4 (14-)	223-D (11-)
	1119(s)	1110	2232-S(49+)	223-4 (19-)	223-4 (17-)	2232-S(10+)
	1062(s)	1058	2232-S(30+)	3223-S(29+)	223-4 (20-)	223-D (10-)
	947(s)	945	223-4 (46-)	2232-S(14-)	3223-S(11-)	
	846(s)	845	2232-S(45-)	223-4 (42-)	223-6 (17-)	223-5 (14-)
	537(s)	541	223-D (52+)	232-B (18-)	2232-S(11-)	
	363(s)	370	223-D (29-)	232-B (21-)	223-D (21-)	3223-S(17-)
	216(s)	213	232-B (37-)	223-D (34+)	3223-T(29-)	
	165(s)	168	2232-T(38+)	3223-T(34+)	223-D (16+)	
		96	2232-T(81-)			

[a] The point group given is that to which the symmetry of the molecular chain is isomorphous. The internal-rotation angles of τ(C–C)=75.3° and τ(C–O)=180.2° were used in the calculation.

Calculated frequencies higher than 2000 cm^{-1}

2965 2965 2964 2963 2868 2867 2862 2862

References

[1] IR. T. Miyazawa, K. Fukushima, and Y. Ideguchi, J. Chem. Phys., **37**, 2764 (1962).

[2] IR. T. Yoshihara, H. Tadokoro, and S. Murahashi, J. Chem. Phys., **41**, 2902 (1964).

[3] R. R. F. Schaufele, Trans. New York Acad. Sci., **30**, 69 (1967).

[4] R. J. L. Koenig and A. C. Angood, J. Polym. Sci., Pt. A-2, **8**, 1787 (1970).

No. 72
Molecule: (32'2') $(OCD_2CD_2)_n$
Symmetry[a] D_7

Sym. species	Observed frequency cm^{-1}	Calculated frequency cm^{-1}	Assignment (P.E.D. %)			
a_1		1278	3223-S(53-)	223-5 (36+)	232-B (12+)	
		1092	223-2 (60+)	2232-S(25+)	223-5 (23+)	
		1008	2232-S(54-)	223-2 (21+)	223-6 (10+)	
		916	223-5 (31+)	223-4 (17-)	3223-S(16+)	223-2 (10-)
		889	223-6 (67+)	223-4 (14-)		
		698	223-4 (52+)	223-5 (29+)	2232-S(27+)	223-6 (15+)
		240	223-D (23+)	3223-S(22+)	232-B (19+)	3223-T(10-)
		209	232-B (46+)	2232-T(24-)	3223-T(17+)	223-D (15-)
a_2	1117(s)	1128	2232-S(84+)	223-5 (50+)		
	1087(s)	1075	223-2 (88+)			
	996(s)	985	223-5 (37-)	223-2 (15-)	2232-S(11+)	223-4 (10-)
	940(s)	948	223-6 (41-)	223-4 (24+)	223-5 (11-)	
	800(s)	796	223-6 (40+)	223-4 (36+)	223-D (24-)	
	453(s)	456	223-D (80+)	223-4 (21+)	223-6 (13+)	223-5 (12-)
	95(s)	101	2232-T(88+)	223-4 (10+)		
e_1	1255(s)	1238	3223-S(54+)	223-5 (39-)		
	1145(s)	1140	2232-S(46+)	223-5 (35+)	2232-S(23+)	223-2 (15+)
	1087(s)	1094	223-2 (55-)	223-5 (19+)	223-2 (10-)	223-5 (10-)
	1050(s)	1066	223-2 (39-)	223-2 (27+)	223-5 (18-)	2232-S(18+)
	1016(s)	1030	2232-S(39-)	2232-S(20+)	223-2 (13+)	
		994	223-5 (39+)	223-2 (14+)	2232-S(11-)	2232-S(9-)
	942(s)	959	223-6 (37+)	223-4 (25-)	223-6 (10+)	
	919(s)	914	223-6 (24-)	3223-S(16+)	223-5 (12+)	223-4 (11-)
	885(s)	881	223-6 (44-)	223-4 (19+)	223-6 (16+)	
	780(s)	771	223-4 (40-)	223-5 (17-)	223-6 (12-)	223-D (10-)
	703(s)	694	223-4 (42-)	223-6 (32-)	2232-S(26-)	223-5 (15-)
	458(s)	467	223-D (39+)	232-B (19-)	223-5 (13-)	
		330	223-D (33+)	232-B (22+)	223-D (18+)	3223-S(15+)
	183(s)	182	223-D (45+)	232-B (37-)	3223-T(18-)	
	156(s)	162	3223-T(48-)	2232-T(36-)		
		85	2232-T(82+)			

[a] The point group given is that to which the symmetry of the molecular chain is isomorphous. The internal-rotation angles of τ(C–C)=75.3° and τ(C–O)=180.2° were used in the calculation.

Calculated frequencies higher than 2000 cm^{-1}

2216 2216 2213 2212 2112 2109 2093 2090

Reference

[1] IR. T. Yoshihara, H. Tadokoro, and S. Murahashi, J. Chem. Phys., **41**, 2902 (1964).

No. 73
Molecule: 1421-T $CH_3SCH_2CH_3$ (trans form)
Symmetry C_s Symmetry number $\sigma = 1$

Sym. species	Observed frequency cm^{-1}	Calculated frequency cm^{-1}	Assignment (P.E.D. %)		
a'	1461*(s)	1464	210-4 (72+)	210-5 (12+)	421-2 (11-)
	1444*	1445	014-4 (69+)	421-2 (14+)	
	1427*	1433	421-2 (40+)	014-4 (25-)	210-2 (21-)
	1377*	1384	210-2 (76+)	421-2 (26+)	
	1320*	1323	014-2 (99+)		
	1267*	1271	421-5 (84+)	210-5 (10+)	
	1065	1060	4210-S(41-)	210-5 (36+)	
	982	983	4210-S(47-)	210-5 (28-)	421-5 (10+)
	960*	964	014-5 (91+)		
	725*	726	0142-S(95+)		
	678	674	1421-S(86-)		
	353*	362	421-D (41+)	142-B (27+)	4210-S(7+)
	211	216	142-B (80+)	421-D (61-)	421-2 (11+)
a"	1455*	1463	210-7 (81+)	210-8 (14+)	
	1427*	1432	014-7 (96+)		
	1251*	1257	421-6 (65+)	210-8 (13-)	210-7 (10+)
	1044*	1037	210-8 (40+)	421-6 (29+)	421-4 (28+)
	955	957	014-8 (94+)		
	785	782	421-4 (65-)	210-8 (37+)	
	273*	254	4210-T(94+)		
		158	0142-T(99+)		
		74	1421-T(98+)		

Calculated frequencies higher than 2000 cm^{-1}

2963 2962 2954 2953 2943 2905 2879 2857

* Weight of the observed frequency is zero.

References

[1] IR. M. Ohsaku, Y. Shiro, and H. Murata, Bull. Chem. Soc. Jpn., **45**, 954 (1972).

[2] R. M. Sakakibara, H. Matsuura, I. Harada, and T. Shimanouchi, Bull. Chem. Soc. Jpn., **50**, 111 (1977).

No. 74
Molecule: 1421-G $CH_3SCH_2CH_3$ (gauche form)
Symmetry C_1 Symmetry number $\sigma = 1$

Sym. species	Observed frequency cm^{-1}	Calculated frequency cm^{-1}	Assignment (P.E.D. %)			
a	1461(s)	1463	210-7 (81+)	210-8 (14+)		
	1455	1462	210-4 (79+)	210-5 (12+)		
	1444	1442	014-4 (96+)			
	1427	1432	014-7 (68+)	421-2 (15+)	210-2 (10-)	
	1427	1431	421-2 (35+)	014-7 (29-)	210-2 (25-)	
	1377	1378	210-2 (68+)	421-2 (36+)		
	1320	1322	014-2 (102+)			
	1267	1274	421-5 (82+)			
	1251	1255	421-6 (66+)	210-8 (12-)		
	1060	1051	210-5 (41+)	4210-S(40-)		
	1044	1026	210-8 (45+)	421-6 (27+)	421-4 (24+)	
	973	984	4210-S(45+)	210-5 (21+)	014-5 (9+)	
	960	964	014-5 (82+)			
	948	957	014-8 (94+)			
	758	763	421-4 (73-)	210-8 (30+)		
	725	725	0142-S(86+)	1421-S(14-)		
	653	656	1421-S(82+)	0142-S(18+)		
	353	348	421-D (65-)	142-B (49+)		
	273	271	142-B (41+)	4210-T(39+)	421-D (20+)	421-4 (13+)
	232	231	4210-T(55-)	142-B (33+)	421-D (11+)	
		155	0142-T(97+)			
		74	1421-T(97+)			

Calculated frequencies higher than 2000 cm^{-1}

2962 2962 2954 2953 2942 2904 2879 2857

References

[1] IR. M. Ohsaku, Y. Shiro, and H. Murata, Bull. Chem. Soc. Jpn., **45**, 954 (1972).

[2] R. M. Sakakibara, H. Matsuura, I. Harada, and T. Shimanouchi, Bull. Chem. Soc. Jpn., **50**, 111 (1977).

No. 75
Molecule: 1'421-T $CD_3SCH_2CH_3$ (trans form)
Symmetry C_s Symmetry number σ = 1

Sym. species	Observed frequency cm^{-1}	Calculated frequency cm^{-1}	Assignment (P.E.D. %)			
a'	1462*(s)	1464	210-4 (74+)	210-5 (12+)		
	1426*	1436	421-2 (55+)	210-2 (25-)	210-4 (10+)	
	1378*	1383	210-2 (77+)	421-2 (26+)		
	1278*	1273	421-5 (87+)	210-5 (10+)		
	1063	1069	4210-S(35-)	210-5 (28+)	014-2 (10+)	
	1049*	1041	014-4 (88+)			
	1013*	1006	014-2 (86+)	0142-S(13+)	210-5 (10-)	
	983	982	4210-S(48-)	210-5 (24-)		
	761	750	014-5 (70+)	1421-S(22-)		
	698*	688	0142-S(79+)			
	648	652	1421-S(63+)	014-5 (25+)		
	345*	351	421-D (47+)	142-B (21+)	4210-S(6+)	
	200	203	142-B (84+)	421-D (54-)	421-2 (11+)	
a"	1454*	1463	210-7 (81+)	210-8 (14+)		
	1266*	1257	421-6 (65+)	210-8 (13-)	210-7 (10+)	
	1040*	1037	210-8 (39+)	421-6 (29+)	421-4 (27+)	
	1040*	1034	014-7 (96+)			
	789*	783	421-4 (64+)	210-8 (37-)		
	720*	718	014-8 (97+)			
	263*	254	4210-T(95+)			
		116	0142-T(99+)			
		72	1421-T(97+)			

Calculated frequencies higher than 2000 cm^{-1}
2963 2962 2943 2905 2879 2205 2202 2053

* Weight of the observed frequency is zero.

References

[1] IR. M. Ohsaku, Y. Shiro, and H. Murata, Bull. Chem. Soc. Jpn., **46**, 1399 (1973).

[2] R. M. Sakakibara, H. Matsuura, I. Harada, and T. Shimanouchi, Bull. Chem. Soc. Jpn., **50**, 111 (1977).

No. 76
Molecule: 1'421-G $CD_3SCH_2CH_3$ (gauche form)
Symmetry C_1 Symmetry number $\sigma = 1$

Sym. species	Observed frequency cm^{-1}	Calculated frequency cm^{-1}	Assignment (P.E.D. %)			
a	1462(s)	1463	210-7 (81+)	210-8 (14+)		
	1454	1462	210-4 (79+)	210-5 (12+)		
	1426	1431	421-2 (50+)	210-2 (36-)		
	1378	1378	210-2 (68+)	421-2 (36+)		
	1278	1275	421-5 (84+)			
	1266	1255	421-6 (66+)	210-8 (12-)		
	1056	1054	4210-S(34-)	210-5 (33+)	014-4 (12+)	
	1049	1043	014-4 (80+)			
	1042(s)	1034	014-7 (97+)			
	1038(s)	1030	210-8 (39+)	421-6 (24+)	421-4 (22+)	014-2 (14+)
	1013	1008	014-2 (74+)	0142-S(12+)		
	971	979	4210-S(50+)	210-5 (22+)		
	789	776	421-4 (47+)	210-8 (22-)	014-5 (21-)	
	728	731	014-5 (54-)	421-4 (27-)	1421-S(13+)	
	720	719	014-8 (97+)			
	698	690	0142-S(63-)	1421-S(21+)		
	639	637	1421-S(58+)	0142-S(29+)	014-5 (12+)	
	345	339	421-D (74+)	142-B (36-)		
	263	265	4210-T(55+)	142-B (34+)	421-4 (13+)	421-D (11+)
	215	223	142-B (49+)	4210-T(39-)	421-D (12+)	
		113	0142-T(96-)			
		70	1421-T(95+)			

Calculated frequencies higher than 2000 cm^{-1}

2962 2962 2942 2904 2879 2205 2202 2053

References

[1] IR. M. Ohsaku, Y. Shiro, and H. Murata, Bull. Chem. Soc. Jpn., **46**, 1399 (1973).

[2] R. M. Sakakibara, H. Matsuura, I. Harada, and T. Shimanouchi, Bull. Chem. Soc. Jpn., **50**, 111 (1977).

No. 77

Molecule: 1421'-T $CH_3SCH_2CD_3$ (trans form)

Symmetry C_s Symmetry number $\sigma = 1$

Sym. species	Observed frequency cm^{-1}	Calculated frequency cm^{-1}	Assignment (P.E.D. %)		
a'	1444*	1444	014-4 (86+)		
	1425*	1423	421-2 (82+)	014-4 (10-)	
	1321*	1323	014-2 (100+)		
	1244	1253	421-5 (95+)	4210-S(12+)	
	1127	1122	210-2 (67+)	4210-S(45+)	
	1052*	1045	210-4 (87+)	210-5 (10+)	
	955*	969	014-5 (85+)		
	932	934	4210-S(35-)	210-2 (32+)	014-5 (5-)
	863	856	210-5 (47-)	1421-S(23+)	210-4 (9+)
	724	725	0142-S(98+)		
	628	628	1421-S(70-)	210-5 (28-)	
	329*	340	142-B (35+)	421-D (32+)	4210-S(7+)
	200	205	142-B (71+)	421-D (68-)	421-2 (11+)
a"	1432*	1432	014-7 (96+)		
	1210*	1218	421-6 (87+)		
	1052*	1043	210-7 (88+)		
	955*	966	421-4 (41+)	014-8 (33-)	210-8 (12+)
	955*	953	014-8 (62+)	421-4 (21+)	
	651*	666	210-8 (70+)	421-4 (32-)	
	200*	193	4210-T(86+)	0142-T(10-)	
		155	0142-T(90+)		
		69	1421-T(97+)		

Calculated frequencies higher than 2000 cm^{-1}

2954 2953 2943 2905 2857 2211 2210 2079

* Weight of the observed frequency is zero.

Reference

[1] R. M. Sakakibara, H. Matsuura, I. Harada, and T. Shimanouchi, Bull. Chem. Soc. Jpn., 50, 111 (1977).

No. 78
Molecule: 1421'-G $CH_3SCH_2CD_3$ (gauche form)
Symmetry C_1 Symmetry number $\sigma = 1$

Sym. species	Observed frequency cm^{-1}	Calculated frequency cm^{-1}	Assignment (P.E.D. %)			
a	1444	1442	014-4 (96+)			
	1432	1432	014-7 (96+)			
	1425	1413	421-2 (91+)			
	1321	1322	014-2 (103+)			
	1263	1257	421-5 (93+)	4210-S(12+)	421-2 (10+)	
	1210	1218	421-6 (87+)			
	1115	1118	210-2 (70+)	4210-S(45+)		
	1060(s)	1045	210-4 (87+)	210-5 (10+)		
	1052	1043	210-7 (89+)			
	985	971	014-5 (79+)			
	955	958	014-8 (93+)			
	924	935	421-4 (39+)	210-8 (15+)	014-5 (12+)	4210-S(9-)
	917	920	4210-S(31+)	210-2 (23-)	421-4 (17+)	
	851	857	210-5 (49+)	1421-S(23-)		
	719	717	0142-S(97+)			
	651	664	210-8 (62+)	421-4 (34-)		
	617	620	1421-S(73+)	210-5 (21+)		
	329	327	142-B (66-)	421-D (49+)	421-4 (10-)	
	258	249	142-B (49+)	421-D (41+)		
	176(s)	176	4210-T(84-)			
		154	0142-T(96+)			
		69	1421-T(96+)			

Calculated frequencies higher than 2000 cm^{-1}

2954 2953 2943 2904 2857 2211 2210 2079

Reference

[1] R. M. Sakakibara, H. Matsuura, I. Harada, and T. Shimanouchi, Bull. Chem. Soc. Jpn., **50**, 111 (1977).

No. 79
Molecule: 142′1′-T $CH_3SCD_2CD_3$ (trans form)
Symmetry C_s Symmetry number $\sigma = 1$

Sym. species	Observed frequency cm^{-1}	Calculated frequency cm^{-1}	Assignment (P.E.D. %)			
a′	1442*	1442	014-4 (96+)			
	1320*	1323	014-2 (103+)			
	1140	1137	4210-S(65+)	210-2 (48+)		
	1067*	1077	421-2 (49+)	421-5 (11-)	210-4 (11-)	210-5 (10-)
	1044*	1038	210-4 (78+)	421-5 (10-)		
	1025*	1030	421-5 (40+)	210-2 (36-)		
	968*	962	014-5 (89+)			
	887*	879	210-5 (27+)	421-2 (19+)	4210-S(17-)	210-2 (13+)
	770*	769	421-5 (33-)	210-5 (24+)	4210-S(13+)	0142-S(6-)
	723	720	0142-S(93-)			
	622	614	1421-S(73-)	210-5 (21-)		
	322*	335	142-B (34+)	421-D (33+)	4210-S(6+)	
	200	203	142-B (71+)	421-D (68-)	421-2 (11+)	
a″	1430*	1432	014-7 (96+)			
	1050*	1043	210-7 (86+)	210-8 (11+)		
	960*	958	014-8 (75+)			
	960*	956	421-6 (27-)	210-8 (24+)	014-8 (20-)	421-4 (10+)
	786*	790	421-6 (55+)	421-4 (29+)	210-8 (16+)	
	576	577	421-4 (55-)	210-8 (46+)	421-6 (11+)	
	200*	188	4210-T(89+)			
		155	0142-T(91+)			
		66	1421-T(98+)			

Calculated frequencies higher than 2000 cm^{-1}
2954 2953 2857 2215 2211 2185 2134 2077

* Weight of the observed frequency is zero.

References

[1] IR. M. Ohsaku, Y. Shiro, and H. Murata, Bull. Chem. Soc. Jpn., **46**, 1399 (1973).

[2] R. M. Sakakibara, H. Matsuura, I. Harada, and T. Shimanouchi, Bull. Chem. Soc. Jpn., **50**, 111 (1977).

No. 80

Molecule: 142'1'-G $CH_3SCD_2CD_3$ (gauche form)

Symmetry C_1 Symmetry number $\sigma = 1$

Sym. species	Observed frequency cm^{-1}	Calculated frequency cm^{-1}	Assignment (P.E.D. %)			
a	1442	1442	014-4 (96+)			
	1430	1432	014-7 (96+)			
	1320	1321	014-2 (104+)			
	1138	1133	4210-S(63+)	210-2 (53+)	421-5 (14+)	
	1067	1064	421-2 (38-)	210-4 (24+)	421-5 (15+)	210-5 (14+)
	1050	1043	210-7 (86+)	210-8 (10+)		
	1044	1040	210-4 (53+)	421-5 (29-)	210-2 (12+)	
	1025	1022	421-2 (45+)	210-2 (21-)	210-4 (14+)	421-5 (10+)
	978	968	014-5 (78+)			
	968	958	014-8 (93+)			
	960	946	421-6 (35-)	210-8 (25+)	014-5 (12+)	
	887	877	210-5 (28+)	4210-S(20-)	210-2 (14+)	421-2 (13+)
	786	788	421-6 (39-)	421-4 (24-)	210-8 (20-)	0142-S(12+)
	770	768	421-5 (31-)	210-5 (21+)	4210-S(10+)	421-6 (7+)
	716	709	0142-S(84+)			
	612	608	1421-S(75+)	210-5 (14+)		
	564	559	421-4 (66+)	210-8 (37-)		
	322	322	142-B (63-)	421-D (52+)		
	244	242	142-B (53+)	421-D (39+)		
	178(s)	176	4210-T(86-)			
		154	0142-T(96+)			
		66	1421-T(97+)			

Calculated frequencies higher than 2000 cm^{-1}

2954 2953 2857 2214 2210 2184 2130 2077

References

[1] IR. M. Ohsaku, Y. Shiro, and H. Murata, Bull. Chem. Soc. Jpn., **46**, 1399 (1973).

[2] R. M. Sakakibara, H. Matsuura, I. Harada, and T. Shimanouchi, Bull. Chem. Soc. Jpn., **50**, 111 (1977).

No. 81
Molecule: 12421-TT $CH_3CH_2SCH_2CH_3$ (trans-trans form)
Symmetry C_{2v} Symmetry number $\sigma = 2$

Sym. species	Observed frequency cm^{-1}	Calculated frequency cm^{-1}	Assignment (P.E.D. %)			
a_1	1463	1466	210-4 (32+)	012-4 (32+)	421-2 (10-)	124-2 (10-)
	1436	1442	124-2 (27+)	421-2 (27+)	012-4 (11+)	210-4 (11+)
	1382	1388	012-2 (43+)	210-2 (43+)		
	1273	1270	124-5 (45+)	421-5 (45-)		
	1077	1075	0124-S(20+)	4210-S(20+)	012-5 (16-)	210-5 (16-)
	994	985	0124-S(21-)	4210-S(21-)	012-5 (16-)	210-5 (16-)
	695	688	1242-S(42-)	2421-S(42-)		
	334	339	242-B (27+)	421-D (13+)	124-D (13+)	1242-S(9+)
	147(s)	153	242-B (78+)	421-D (38-)	124-D (38-)	
a_2	1456	1463	012-7 (41+)	210-7 (41+)		
	1252	1255	421-6 (32+)	124-6 (32+)	210-8 (7-)	
	1026(s)	1032	210-8 (20+)	012-8 (20+)	421-6 (15+)	124-6 (15+)
	782	778	421-4 (33-)	124-4 (33+)	210-8 (18+)	012-8 (18+)
	260	251	4210-T(47+)	0124-T(47+)		
		85	1242-T(49+)	2421-T(49+)		
b_1	1463	1462	012-4 (39-)	210-4 (39+)		
	1431	1431	421-2 (25+)	124-2 (25-)	210-2 (17-)	012-2 (17+)
	1375	1378	210-2 (34-)	012-2 (34+)	421-2 (17-)	124-2 (17+)
	1278	1273	421-5 (42+)	124-5 (42+)		
	1047	1047	4210-S(21-)	0124-S(21+)	210-5 (21+)	012-5 (21-)
	979	979	4210-S(25+)	0124-S(25-)	210-5 (14+)	012-5 (14-)
	689	681	2421-S(48-)	1242-S(48+)		
	349	349	124-D (52-)	421-D (52+)		
b_2	1456	1463	210-7 (41+)	012-7 (41-)		
	1260	1258	124-6 (33+)	421-6 (33-)	012-8 (6-)	
	1047	1041	012-8 (20-)	210-8 (20+)	124-4 (15+)	421-4 (15+)
	797	787	124-4 (32+)	421-4 (32+)	012-8 (19+)	210-8 (19-)
	260	256	0124-T(48-)	4210-T(48+)		
		54	1242-T(49+)	2421-T(49-)		

Calculated frequencies higher than 2000 cm^{-1}

2963 2963 2962 2962 2943 2943 2907 2904 2879 2879

Reference

[1] IR.R. M. Ohta, Y. Ogawa, H. Matsuura, I. Harada, and T. Shimanouchi, Bull. Chem. Soc. Jpn., **50**, 380 (1977).

No. 82
Molecule: 12421-TG $CH_3CH_2SCH_2CH_3$ (trans-gauche form)
Symmetry C_1 Symmetry number σ = 1

Sym. species	Observed frequency cm^{-1}	Calculated frequency cm^{-1}	Assignment (P.E.D. %)			
a	1463*	1464	012-4 (60-)	210-7 (11-)	012-5 (10-)	
	1463*	1463	012-7 (81+)	012-8 (14+)		
	1456*	1463	210-7 (68+)	210-8 (12+)		
	1456*	1462	210-4 (72+)	210-5 (11+)		
	1436*	1436	124-2 (54-)	012-2 (25+)	012-4 (10-)	
	1431*	1431	421-2 (49+)	210-2 (36-)		
	1382*	1383	012-2 (76-)	124-2 (25-)		
	1375*	1377	210-2 (66+)	421-2 (35+)		
	1278*	1277	421-5 (51+)	124-5 (31+)		
	1278*	1271	124-5 (52-)	421-5 (32+)		
	1260*	1257	124-6 (62-)	012-8 (12+)		
	1252*	1254	421-6 (60+)	210-8 (11-)		
	1077*	1065	0124-S(36-)	012-5 (29+)	4210-S(6+)	
	1047*	1050	210-5 (35+)	4210-S(32-)	210-4 (6-)	
	1032	1037	012-8 (38+)	124-6 (28+)	124-4 (26-)	
	1018	1026	210-8 (44-)	421-6 (26-)	421-4 (23-)	
	979*	983	0124-S(31-)	012-5 (24-)	4210-S(11+)	124-5 (8-)
	979*	980	4210-S(40-)	210-5 (19-)	0124-S(13-)	
	782*	783	124-4 (65+)	012-8 (37+)		
	766	762	421-4 (73+)	210-8 (30-)		
	695*	686	1242-S(54-)	2421-S(40+)		
	658	663	2421-S(53-)	1242-S(37-)		
	384	381	421-D (31+)	242-B (30-)	124-D (22-)	
	307	299	421-D (59-)	124-D (30-)		
	260*	259	4210-T(67+)	0124-T(13+)	242-B (13+)	124-D (10-)
	243	252	0124-T(80-)	4210-T(13+)		
	187	187	242-B (74+)	124-D (37-)	4210-T(14-)	
		70	2421-T(67+)	1242-T(29+)		
		64	1242-T(67-)	2421-T(28+)		

Calculated frequencies higher than 2000 cm^{-1}

2963 2962 2962 2962 2943 2942 2906 2904 2879 2879

* Weight of the observed frequency is zero.

Reference

[1] IR.R. M. Ohta, Y. Ogawa, H. Matsuura, I. Harada, and T. Shimanouchi, Bull. Chem. Soc. Jpn., **50**, 380 (1977).

No. 83
Molecule: 12421-GG $CH_3CH_2SCH_2CH_3$ (gauche-gauche form)
Symmetry C_2 Symmetry number $\sigma = 2$

Sym. species	Observed frequency cm^{-1}	Calculated frequency cm^{-1}	Assignment (P.E.D. %)			
a	1463*	1462	012-7 (41+)	210-7 (41+)		
	1456*	1462	012-4 (40+)	210-4 (40+)		
	1431*	1430	124-2 (25-)	421-2 (25-)	012-2 (18+)	210-2 (18+)
	1375*	1377	012-2 (34+)	210-2 (34+)	124-2 (19+)	421-2 (19+)
	1278*	1276	421-5 (41+)	124-5 (41-)		
	1252*	1252	421-6 (33+)	124-6 (33+)	210-8 (6-)	
	1047*	1053	0124-S(22-)	4210-S(22-)	012-5 (20+)	210-5 (20+)
	1018*	1017	210-8 (26+)	012-8 (26+)	421-6 (13+)	124-6 (13+)
	979*	979	4210-S(23+)	0124-S(23+)	210-5 (15+)	012-5 (15+)
	739	744	421-4 (41+)	124-4 (41-)	210-8 (12-)	012-8 (12-)
	641	639	2421-S(50+)	1242-S(50+)		
	370	363	242-B (64+)	124-D (32-)	421-D (32-)	
	260*	255	0124-T(33-)	4210-T(33-)	242-B (18-)	
		205	242-B (58-)	4210-T(14+)	0124-T(14+)	421-D (11-)
		48	1242-T(49+)	2421-T(49+)		
b	1463*	1463	210-7 (41-)	012-7 (41+)		
	1456*	1462	210-4 (40-)	012-4 (40+)		
	1431*	1432	421-2 (25+)	124-2 (25-)	210-2 (18-)	012-2 (18+)
	1375*	1378	210-2 (34-)	012-2 (34+)	421-2 (18-)	124-2 (18+)
	1278*	1274	124-5 (42+)	421-5 (42+)		
	1260*	1257	124-6 (32-)	421-6 (32+)	012-8 (6+)	210-8 (6-)
	1047*	1051	210-5 (22+)	012-5 (22-)	4210-S(18-)	0124-S(18+)
	1032*	1038	012-8 (20-)	210-8 (20+)	124-6 (14-)	421-6 (14+)
	979*	983	0124-S(28+)	4210-S(28-)	012-5 (11+)	210-5 (11-)
	782*	783	124-4 (32+)	421-4 (32+)	012-8 (18+)	210-8 (18-)
	695*	689	1242-S(46+)	2421-S(46-)		
	315	322	421-D (45+)	124-D (45-)		
	243*	251	4210-T(45+)	0124-T(45-)		
		85	2421-T(48-)	1242-T(48+)		

Calculated frequencies higher than 2000 cm^{-1}

2963 2962 2962 2962 2943 2941 2904 2904 2879 2879

* Weight of the observed frequency is zero.

Reference

[1] IR.R. M. Ohta, Y. Ogawa, H. Matsuura, I. Harada, and T. Shimanouchi, Bull. Chem. Soc. Jpn., **50**, 380 (1977).

No. 84

Molecule: **14221-TT** **$CH_3SCH_2CH_2CH_3$ (trans-trans form)**

Symmetry C_s **Symmetry number $\sigma = 1$**

Sym. species	Observed frequency cm^{-1}	Calculated frequency cm^{-1}	Assignment (P.E.D. %)			
a′	1468(s)	1482	221-2 (71+)	210-4 (16+)		
	1461(s)	1456	210-4 (67+)	221-2 (22-)		
	1438(s)	1444	014-4 (86+)			
	1420(s)	1423	422-2 (79-)	014-4 (10+)		
	1374(s)	1379	210-2 (104+)			
	1336(s)	1331	221-5 (53+)	014-2 (24+)	4221-S(14-)	422-5 (14-)
	1317(s)	1319	014-2 (78+)	221-5 (21-)		
	1250(s)	1237	422-5 (85+)			
	1102(s)	1095	4221-S(30-)	210-5 (23+)	221-5 (19-)	
	1037(s)	1030	2210-S(81-)	4221-S(17+)		
	962(s)	966	014-5 (91+)			
	902(s)	903	210-5 (39-)	4221-S(35-)	2210-S(11-)	
	762(s)	751	1422-S(76-)			
	718(s)	721	0142-S(98+)			
	354(s)	357	221-D (60-)	142-B (16+)	1422-S(13-)	
	315(s)	329	142-B (41+)	422-D (26+)	4221-S(7+)	
	159(s)	156	422-D (68-)	142-B (51+)	221-D (23+)	
a″	1451(s)	1463	210-7 (81+)	210-8 (14+)		
	1437(s)	1432	014-7 (96+)			
	1293(s)	1295	221-6 (56+)	422-6 (23-)		
	1242(s)	1225	422-6 (41+)	210-8 (17-)	221-4 (14-)	221-6 (11+)
	1053(s)	1070	422-6 (31+)	422-4 (18+)	210-8 (18+)	221-4 (15+)
	962(s)	957	014-8 (95+)			
	864(s)	855	422-4 (45+)	210-8 (39-)	221-6 (21-)	
	751(s)	738	221-4 (58-)	422-4 (28+)	210-8 (13+)	
		228	2210-T(95+)			
		162	0142-T(92+)			
		111	4221-T(83-)			
		70	1422-T(97+)			

Calculated frequencies higher than 2000 cm^{-1}

2962 2962 2954 2953 2944 2906 2904 2880 2868 2857

References

[1] IR.R. N. Nogami, H. Sugeta, and T. Miyazawa, Chem. Lett., **1975**, 147.

[2] IR.R. N. Nogami, unpublished work.

No. 85

Molecule: 14221-TG $CH_3SCH_2CH_2CH_3$ (trans-gauche form)

Symmetry C_1 Symmetry number $\sigma = 1$

Sym. species	Observed frequency cm^{-1}	Calculated frequency cm^{-1}	Assignment (P.E.D. %)			
a		1479	221-2 (69+)	210-4 (17+)		
	1457*	1463	210-7 (77+)	210-8 (14+)		
	1457*	1457	210-4 (65+)	221-2 (19-)		
	1442*	1451	422-2 (38+)	014-4 (23+)	221-5 (12-)	422-5 (10-)
	1431*	1439	014-4 (73+)	422-2 (11-)		
	1431*	1432	014-7 (96+)			
	1379*	1384	221-5 (30+)	422-2 (29+)	210-2 (17+)	422-5 (11+)
	1379*	1379	210-2 (89+)			
	1321*	1322	014-2 (101+)			
	1296*	1298	221-6 (49+)	422-6 (21+)	422-2 (6+)	
	1214	1217	422-5 (32+)	210-8 (14+)	422-6 (13+)	4221-S(10+)
		1192	422-6 (32-)	422-5 (20+)	4221-S(17+)	210-5 (17-)
	1090*	1095	4221-S(23+)	2210-S(17-)	210-8 (13-)	221-4 (13-)
	1073*	1064	210-5 (24+)	2210-S(20-)	422-4 (16-)	422-6 (15-)
	1032*	1029	2210-S(19-)	422-5 (15-)	210-8 (12+)	221-6 (11+)
	958*	966	014-5 (91-)			
	958*	957	014-8 (95-)			
	895*	885	4221-S(36+)	210-5 (30+)	2210-S(17+)	
	850*	844	422-4 (54+)	2210-S(21-)		
	791	787	221-4 (44+)	210-8 (33-)	1422-S(10-)	
	723*	725	0142-S(95+)			
	667	670	1422-S(74+)	221-4 (14+)		
	428*	442	221-D (48-)	422-D (17+)	1422-S(8+)	
	292	289	221-D (31-)	142-B (27-)	422-D (12-)	2210-T(9-)
	236*	246	2210-T(49+)	142-B (47-)	422-D (12+)	
		176	422-D (43-)	2210-T(36+)	142-B (22+)	4221-T(11+)
		158	0142-T(91-)			
		106	4221-T(65-)	422-D (18-)		
		54	1422-T(93+)			

Calculated frequencies higher than 2000 cm^{-1}

2963 2962 2954 2953 2944 2907 2903 2880 2868 2857

* Weight of the observed frequency is zero.

References

[1] IR.R. N. Nogami, H. Sugeta, and T. Miyazawa, Chem. Lett., **1975**, 147.

[2] IR.R. N. Nogami, unpublished work.

No. 86
Molecule: 14221-GT $CH_3SCH_2CH_2CH_3$ (gauche-trans form)
Symmetry C_1 Symmetry number $\sigma = 1$

Sym. species	Observed frequency cm^{-1}	Calculated frequency cm^{-1}	Assignment (P.E.D. %)			
a	1470(s)	1482	221-2 (72+)	210-4 (16+)		
	1464(s)	1463	210-7 (81+)	210-8 (14+)		
	1454(s)	1456	210-4 (69+)	221-2 (21-)		
	1448(s)	1442	014-4 (96+)			
	1428(s)	1432	014-7 (96+)			
	1416(s)	1412	422-2 (88-)			
	1367(s)	1379	210-2 (104+)			
	1341(s)	1330	221-5 (63-)	4221-S(16+)	422-5 (13+)	014-2 (12+)
	1321(s)	1320	014-2 (91-)	221-5 (10-)		
	1295(s)	1293	221-6 (56+)	422-6 (23-)		
	1242(s)	1240	422-5 (81+)			
	1223(s)	1225	422-6 (43+)	210-8 (16-)	221-4 (13-)	221-6 (10+)
	1090(s)	1089	4221-S(30-)	210-5 (25+)	221-5 (20-)	
	1075(s)	1063	422-6 (29+)	210-8 (20+)	221-6 (17+)	221-4 (16+)
	1031(s)	1031	2210-S(81-)	4221-S(16+)		
	958(s)	968	014-5 (90+)			
	958(s)	957	014-8 (95+)			
	898(s)	896	4221-S(38+)	210-5 (36+)	2210-S(11+)	
	840(s)	837	422-4 (42-)	210-8 (40+)	221-6 (18+)	221-4 (14-)
	747(s)	758	1422-S(58-)	0142-S(26+)		
	730(s)	731	221-4 (48-)	422-4 (38+)		
	697(s)	698	0142-S(77+)	1422-S(22+)		
	374(s)	375	221-D (28+)	142-B (26-)	422-D (20+)	1422-S(12+)
	285(s)	290	142-B (74-)	221-D (30-)		
	236	231	2210-T(61+)	422-D (25+)	221-D (12-)	
		213	422-D (35+)	2210-T(29-)	142-B (21+)	221-D (11-)
		151	0142-T(90+)			
		99	4221-T(85-)			
		69	1422-T(95-)			

Calculated frequencies higher than 2000 cm^{-1}

2962 2962 2954 2953 2943 2905 2904 2880 2869 2857

References

[1] IR.R. N. Nogami, H. Sugeta, and T. Miyazawa, Chem. Lett., **1975**, 147.
[2] IR.R. N. Nogami, unpublished work.

No. 87
Molecule: 14221-GG $CH_3SCH_2CH_2CH_3$ (gauche-gauche form)
Symmetry C_1 Symmetry number $\sigma = 1$

Sym. species	Observed frequency cm^{-1}	Calculated frequency cm^{-1}	Assignment (P.E.D. %)			
a	1468*(s)	1479	221-2 (68+)	210-4 (19+)		
	1456*(s)	1463	210-7 (80+)	210-8 (14+)		
	1456*(s)	1457	210-4 (63+)	221-2 (21-)		
	1442*	1442	014-4 (87+)			
	1426*(s)	1441	422-2 (40-)	422-5 (16+)	221-5 (16+)	
	1426*(s)	1432	014-7 (96+)			
	1377*(s)	1380	210-2 (94+)			
	1377*(s)	1376	422-2 (40+)	221-5 (28+)	210-2 (12-)	
	1318(s)	1321	014-2 (103+)			
	1300(s)	1297	221-6 (49+)	422-6 (22+)		
	1221(s)	1221	422-5 (35+)	4221-S(14+)	210-8 (12+)	422-6 (11+)
		1192	422-6 (36-)	422-5 (17+)	210-5 (16-)	4221-S(15+)
	1093(s)	1090	4221-S(23-)	2210-S(19+)	210-8 (16+)	221-4 (14+)
	1063(s)	1059	210-5 (27+)	2210-S(18-)	422-6 (15-)	422-4 (14-)
	1039(s)	1029	2210-S(20-)	422-5 (15-)	4221-S(12+)	210-8 (11+)
	963(s)	967	014-5 (91+)			
	954(s)	957	014-8 (95-)			
	888(s)	877	4221-S(42+)	210-5 (26+)	2210-S(23+)	
	831(s)	825	422-4 (54+)	210-8 (16+)	2210-S(11-)	221-4 (10-)
	781(s)	781	221-4 (38+)	210-8 (26-)	422-4 (20+)	
	724(s)	723	0142-S(87-)			
	648(s)	656	1422-S(75+)	0142-S(16+)		
	429(s)	426	221-D (57+)	422-D (23-)		
	339(s)	331	142-B (74-)	422-D (23+)		
	236	232	2210-T(55-)	142-B (36-)		
		181	422-D (43-)	2210-T(27+)	221-D (15-)	142-B (11-)
		156	0142-T(85+)			
		113	4221-T(62-)	1422-T(12+)		
		50	1422-T(83+)	4221-T(14+)		

Calculated frequencies higher than 2000 cm^{-1}

2963 2962 2954 2953 2943 2906 2903 2880 2868 2857

* Weight of the observed frequency is zero.

References

[1] IR.R. N. Nogami, H. Sugeta, and T. Miyazawa, Chem. Lett., **1975**, 147.
[2] IR.R. N. Nogami, unpublished work.

No. 88

Molecule: 124221-TTT **$CH_3CH_2SCH_2CH_2CH_3$ (trans-trans-trans form)**

Symmetry C_s **Symmetry number σ = 1**

Sym. species	Observed frequency cm^{-1}	Calculated frequency cm^{-1}	Assignment (P.E.D. %)			
a′	1473	1482	221-2 (71+)	210-4 (16+)		
	1465	1464	012-4 (69+)	124-2 (12-)	012-5 (11+)	
	1449	1456	210-4 (66+)	221-2 (21-)		
	1440	1441	124-2 (43+)	422-2 (18+)	012-2 (14-)	012-4 (14+)
	1423	1422	422-2 (65+)	012-2 (15+)		
	1375	1382	012-2 (73+)	124-2 (26+)		
	1375	1379	210-2 (104+)			
	1335	1328	221-5 (74-)	4221-S(17+)	422-5 (13+)	
	1266	1272	124-5 (87+)	012-5 (10-)		
	1239	1238	422-5 (85+)			
	1100	1099	4221-S(27-)	210-5 (20+)	221-5 (17-)	210-4 (7-)
	1047	1058	0124-S(38-)	012-5 (34+)		
	1036	1030	2210-S(81-)	4221-S(16+)		
	981	983	0124-S(45+)	012-5 (30+)	124-5 (10+)	
	899	903	210-5 (39-)	4221-S(34-)	2210-S(10-)	
	764	754	2422-S(79-)			
	693	682	1242-S(90-)			
	392	404	221-D (33-)	124-D (28+)	242-B (11+)	
	307	307	422-D (27+)	242-B (24+)	2422-S(10+)	1242-S(8+)
	277	281	124-D (52-)	221-D (40-)	422-D (10+)	
		113	242-B (65+)	422-D (54-)	124-D (23-)	221-D (13+)
a″	1452	1463	210-7 (81+)	210-8 (14+)		
	1452	1463	012-7 (81+)	012-8 (14+)		
	1298	1295	221-6 (56+)	422-6 (23-)		
	1266	1257	124-6 (65+)	012-8 (13-)	012-7 (10+)	
	1213	1225	422-6 (41+)	210-8 (17-)	221-4 (14-)	221-6 (10+)
	1076	1070	422-6 (31+)	422-4 (18+)	210-8 (18+)	221-4 (15+)
	1023	1036	012-8 (39-)	124-6 (29-)	124-4 (27+)	
	862	855	422-4 (45+)	210-8 (39-)	221-6 (21-)	
	788	783	124-4 (65+)	012-8 (37+)		
	740	738	221-4 (58-)	422-4 (28+)	210-8 (13+)	
	250(s)	254	0124-T(95-)			
	225	228	2210-T(94+)			
		121	4221-T(77+)	1242-T(13-)		
		78	2422-T(52+)	1242-T(35+)	4221-T(10+)	
		48	1242-T(50-)	2422-T(43+)		

Calculated frequencies higher than 2000 cm^{-1}

2963 2962 2962 2962 2944 2943 2907 2904 2904 2880
2879 2869

Reference

[1] IR.R. M. Ohta, Y. Ogawa, H. Matsuura, I. Harada, and T. Shimanouchi, Bull. Chem. Soc. Jpn., **50**, 380 (1977).

No. 89
Molecule: 124221-TGT $CH_3CH_2SCH_2CH_2CH_3$ (trans-gauche-trans form)
Symmetry C_1 Symmetry number $\sigma = 1$

Sym. species	Observed frequency cm^{-1}	Calculated frequency cm^{-1}	Assignment (P.E.D. %)			
a	1473*	1482	221-2 (72+)	210-4 (16+)		
	1465*	1464	012-4 (72+)	012-5 (11+)		
	1452*	1463	210-7 (78+)	210-8 (14+)		
	1452*	1463	012-7 (81+)	012-8 (14+)		
	1449*	1456	210-4 (69+)	221-2 (21-)		
	1440*	1436	124-2 (55+)	012-2 (25-)	012-4 (10+)	
	1417	1412	422-2 (87-)			
	1375*	1383	012-2 (76+)	124-2 (26+)		
	1375*	1379	210-2 (103+)			
	1335*	1329	221-5 (73-)	4221-S(18+)	422-5 (14+)	
	1298*	1294	221-6 (55+)	422-6 (23-)		
	1270	1272	124-5 (85+)			
	1266*	1257	124-6 (65+)	012-8 (13-)	012-7 (10+)	
	1250	1240	422-5 (81+)			
	1219	1225	422-6 (43-)	210-8 (16+)	221-4 (13+)	221-6 (10-)
	1092	1090	4221-S(29-)	210-5 (25+)	221-5 (20-)	
	1076*	1065	422-6 (23-)	210-8 (14-)	422-4 (13-)	221-6 (12-)
	1056	1060	0124-S(29+)	012-5 (27-)	210-8 (7-)	422-6 (6-)
	1036*	1037	012-8 (39+)	124-6 (29+)	124-4 (27-)	
	1030	1031	2210-S(80-)	4221-S(16+)		
	981*	983	0124-S(43+)	012-5 (31+)	124-5 (11+)	
	892	897	4221-S(39+)	210-5 (36+)	2210-S(11+)	
	836	837	422-4 (42-)	210-8 (40+)	221-6 (18+)	221-4 (14-)
	780	783	124-4 (65+)	012-8 (37+)		
	740	748	2422-S(72+)			
	723*	730	221-4 (46+)	422-4 (38-)		
	675	672	1242-S(87+)			
	411	414	242-B (21-)	124-D (19-)	221-D (18+)	422-D (13+)
	307*	309	221-D (30-)	124-D (23-)	2422-S(18-)	
	255	257	0124-T(68-)	422-D (15-)	221-D (10+)	
	245	248	124-D (27+)	422-D (25+)	0124-T(24-)	242-B (24-)
	225	229	2210-T(76+)	422-D (13+)		
	200	189	242-B (51-)	124-D (22+)	422-D (21-)	422-4 (11-)
		89	4221-T(77-)			
		67	2422-T(48+)	1242-T(44+)		
		57	1242-T(49-)	2422-T(42+)		

Calculated frequencies higher than 2000 cm^{-1}
2963 2962 2962 2962 2943 2943 2906 2904 2904 2880
2879 2869

* Weight of the observed frequency is zero.

Reference

[1] IR.R. M. Ohta, Y. Ogawa, H. Matsuura, I. Harada, and T. Shimanouchi, Bull. Chem. Soc. Jpn., **50**, 380 (1977).

No. 90

Molecule: 124221-GTT $CH_3CH_2SCH_2CH_2CH_3$ **(gauche-trans-trans form)**

Symmetry C_1 **Symmetry number** $\sigma = 1$

Sym. species	Observed frequency cm⁻¹	Calculated frequency cm⁻¹	Assignment (P.E.D. %)			
a	1473*	1482	221-2 (71+)	210-4 (16+)		
	1465*	1463	210-7 (81+)	210-8 (14+)		
	1452*	1463	012-7 (81+)	012-8 (14+)		
	1452*	1462	012-4 (79+)	012-5 (12+)		
	1449*	1456	210-4 (68+)	221-2 (21-)		
	1440*	1431	124-2 (50-)	012-2 (35+)		
	1423*	1424	422-2 (87-)			
	1375*	1379	210-2 (102+)			
	1375*	1377	012-2 (66+)	124-2 (35+)		
	1335*	1329	221-5 (73-)	4221-S(17+)	422-5 (14+)	
	1298*	1295	221-6 (56-)	422-6 (23+)		
	1270*	1275	124-5 (83+)			
	1266*	1256	124-6 (63+)	012-8 (12-)		
	1239*	1237	422-5 (82+)			
	1219*	1225	422-6 (41+)	210-8 (17-)	221-4 (14-)	221-6 (10+)
	1100*	1097	4221-S(30-)	210-5 (22+)	221-5 (19-)	
	1076*	1070	422-6 (31+)	422-4 (18+)	210-8 (18+)	221-4 (15+)
	1056*	1051	012-5 (40+)	0124-S(39-)		
	1030*	1031	2210-S(65-)	4221-S(13+)		
	1023*	1025	012-8 (38+)	124-6 (22+)	124-4 (19-)	2210-S(16+)
	972	981	0124-S(50-)	012-5 (25-)	124-5 (10-)	
	899*	905	210-5 (40-)	4221-S(33-)	2210-S(10-)	
	852*	855	422-4 (46+)	210-8 (39-)	221-6 (21-)	
	764*	762	124-4 (70+)	012-8 (28+)		
	740*	749	2422-S(76-)			
	740*	738	221-4 (58+)	422-4 (28-)	210-8 (13-)	
	670	672	1242-S(93+)			
	372	373	242-B (44+)	124-D (34-)	221-D (32-)	
	355	350	221-D (25+)	2422-S(19+)	422-D (18+)	124-D (14-)
	285	279	124-D (43+)	242-B (15+)	422-D (12+)	0124-T(12+)
	245*	247	0124-T(78-)			
	225*	228	2210-T(95+)			
		143	422-D (54+)	242-B (54-)	221-D (17-)	
		118	4221-T(77+)			
		63	2422-T(71+)	1242-T(21+)		
		57	1242-T(62-)	2422-T(24+)		

Calculated frequencies higher than 2000 cm^{-1}

2963 2962 2962 2962 2944 2942 2906 2904 2904 2880
2879 2869

* Weight of the observed frequency is zero.

Reference

[1] IR.R. M. Ohta, Y. Ogawa, H. Matsuura, I. Harada, and T. Shimanouchi, Bull. Chem. Soc. Jpn., **50**, 380 (1977).

No. 91
Molecule: 124221-GGT $CH_3CH_2SCH_2CH_2CH_3$ (gauche-gauche-trans form)
Symmetry C_1 Symmetry number $\sigma = 1$

Sym. species	Observed frequency cm^{-1}	Calculated frequency cm^{-1}	Assignment (P.E.D. %)			
a	1473*	1482	221-2 (72+)	210-4 (16+)		
	1465*	1463	210-7 (79+)	210-8 (14+)		
	1452*	1463	012-7 (79+)	012-8 (13+)		
	1452*	1462	012-4 (79+)	012-5 (12+)		
	1449*	1456	210-4 (69+)	221-2 (21-)		
	1440*	1431	124-2 (50-)	012-2 (36+)		
	1417*	1412	422-2 (88-)			
	1375*	1379	210-2 (104+)			
	1375*	1377	012-2 (67+)	124-2 (36+)		
	1335*	1329	221-5 (73-)	4221-S(18+)	422-5 (14+)	
	1298*	1293	221-6 (56+)	422-6 (23-)		
	1270*	1275	124-5 (83+)			
	1266*	1255	124-6 (64+)	012-8 (12-)		
	1248*	1240	422-5 (80+)			
	1219*	1225	422-6 (43+)	210-8 (16-)	221-4 (13-)	221-6 (10+)
	1092*	1090	4221-S(30-)	210-5 (25+)	221-5 (20-)	
	1076*	1066	422-6 (28+)	210-8 (19+)	422-4 (16+)	221-6 (16+)
	1056*	1052	012-5 (41+)	0124-S(39-)		
	1030*	1031	2210-S(78-)	4221-S(15+)		
	1023*	1026	012-8 (43+)	124-6 (25+)	124-4 (22-)	
	972*	981	0124-S(50-)	012-5 (26-)	124-5 (10-)	
	899*	897	4221-S(38-)	210-5 (36-)	2210-S(12-)	
	836	841	422-4 (41+)	210-8 (37-)	221-6 (18-)	221-4 (11+)
	764*	765	124-4 (52+)	012-8 (22+)	221-4 (13-)	
	740	745	2422-S(63-)	124-4 (10+)		
	723	726	422-4 (40-)	221-4 (39+)		
	658	656	1242-S(89+)			
	383	386	242-B (42-)	221-D (21+)	422-D (16+)	124-D (15+)
	321	330	124-D (58-)	221-D (14+)	242-B (14+)	
	285	275	242-B (38-)	221-D (26-)	0124-T(17-)	124-D (14-)
	240	243	0124-T(71+)	422-D (11+)		
	225*	229	2210-T(77+)	422-D (14+)		
	200	192	242-B (41+)	422-D (33+)		
		102	4221-T(63+)	1242-T(17+)		
		75	2422-T(48-)	1242-T(29+)	4221-T(19-)	
		42	1242-T(49+)	2422-T(44+)		

Calculated frequencies higher than 2000 cm^{-1}
2963 2962 2962 2962 2943 2942 2905 2904 2904 2880
2879 2869

* Weight of the observed frequency is zero.

Reference

[1] IR.R. M. Ohta, Y. Ogawa, H. Matsuura, I. Harada, and T. Shimanouchi, Bull. Chem. Soc. Jpn., **50**, 380 (1977).

No. 92
Molecule: 124221-GGG $CH_3CH_2SCH_2CH_2CH_3$ (gauche-gauche-gauche form)
Symmetry C_1 Symmetry number σ = 1

Sym. species	Observed frequency cm^{-1}	Calculated frequency cm^{-1}	Assignment (P.E.D. %)			
a	1473*	1479	221-2 (68+)	210-4 (19+)		
	1465*	1463	210-7 (79+)	210-8 (14+)		
	1452*	1463	012-7 (81+)	012-8 (14+)		
	1452*	1462	012-4 (80+)	012-5 (12+)		
	1449*	1457	210-4 (63+)	221-2 (21-)		
	1440*	1441	422-2 (45-)	422-5 (18+)	221-5 (17+)	
	1423*	1431	124-2 (50-)	012-2 (36+)		
	1375*	1380	210-2 (95+)			
	1375*	1377	012-2 (67+)	124-2 (36+)		
	1375*	1376	422-2 (41+)	221-5 (29+)	210-2 (11-)	
	1298*	1298	221-6 (49+)	422-6 (22+)		
	1270*	1275	124-5 (83+)			
	1266*	1255	124-6 (66+)	012-8 (12-)		
	1219*	1221	422-5 (35+)	4221-S(14+)	210-8 (12+)	422-6 (11+)
		1192	422-6 (36-)	422-5 (17+)	210-5 (16-)	4221-S(15+)
	1092	1091	4221-S(22-)	2210-S(18+)	210-8 (16+)	221-4 (15+)
	1056*	1061	210-5 (24+)	2210-S(18-)	422-6 (14-)	422-4 (14-)
	1047*	1052	012-5 (40+)	0124-S(38-)		
	1030*	1030	422-5 (13-)	2210-S(12-)	221-5 (11+)	012-8 (10+)
	1023*	1025	012-8 (34-)	124-6 (20-)	124-4 (17+)	
	972*	981	0124-S(50-)	012-5 (26-)	124-5 (10-)	
	892*	878	4221-S(41-)	210-5 (26-)	2210-S(22-)	
	836*	831	422-4 (50+)	210-8 (13+)	2210-S(12-)	
	788*	782	221-4 (42+)	210-8 (29-)	422-4 (11+)	
	764*	756	124-4 (64-)	012-8 (23-)	422-4 (12+)	
	693*	687	1242-S(47-)	2422-S(39+)		
	636	640	1242-S(49+)	2422-S(46+)		
	432	426	221-D (57-)	422-D (23+)	422-4 (10-)	
	363	359	242-B (64+)	124-D (46-)		
	295	297	124-D (43-)	422-D (19+)	242-B (12-)	221-D (10+)
	255*	251	0124-T(73-)	2210-T(11-)		
	213	216	2210-T(53-)	242-B (29-)	0124-T(13+)	
		169	422-D (42-)	242-B (30-)	2210-T(17+)	221-D (13-)
		118	4221-T(57-)	1242-T(10-)	2422-T(10+)	
		63	1242-T(69+)	4221-T(17-)		
		35	2422-T(76+)	1242-T(17+)		

Calculated frequencies higher than 2000 cm^{-1}

2963 2963 2962 2962 2943 2942 2906 2904 2903 2880
2879 2868

* Weight of the observed frequency is zero.

Reference

[1] IR.R. M. Ohta, Y. Ogawa, H. Matsuura, I. Harada, and T. Shimanouchi, Bull. Chem. Soc. Jpn., **50**, 380 (1977).

No. 93
Molecule: 142221-TTT $CH_3SCH_2CH_2CH_2CH_3$ (trans-trans-trans form)
Symmetry C_s Symmetry number σ = 1

Sym. species	Observed frequency cm^{-1}	Calculated frequency cm^{-1}	Assignment (P.E.D. %)			
a′	1476(s)	1487	222-2 (46-)	221-2 (33+)	210-4 (11+)	
	1464	1465	222-2 (47+)	221-2 (22+)	210-4 (21+)	
	1452	1453	210-4 (52-)	221-2 (36+)		
	1445	1444	014-4 (86+)			
	1418	1422	422-2 (78+)			
	1378	1379	210-2 (105+)			
	1354	1355	221-5 (52+)	222-5 (34-)	2221-S(15-)	
	1324	1323	014-2 (98+)			
	1296	1291	222-5 (35+)	422-5 (30-)	221-5 (24+)	
	1227	1223	422-5 (62+)	222-5 (25+)		
	1108	1102	210-5 (22+)	2221-S(20-)	222-5 (9-)	221-5 (9-)
	1053	1056	2221-S(30-)	4222-S(29+)	2210-S(23+)	
	1012	1017	2210-S(55+)	4222-S(36-)		
	968	966	014-5 (90+)			
	897	901	210-5 (42-)	2221-S(31-)	221-5 (10+)	
	765	750	1422-S(74+)	0142-S(10-)		
	719	719	0142-S(92+)			
	425	442	221-D (44-)	142-B (19+)	422-D (12+)	222-D (10-)
	320	320	222-D (33-)	422-D (26-)	1422-S(15-)	
	250	256	142-B (60+)	221-D (31+)		
		119	422-D (63-)	222-D (36+)	142-B (28+)	221-D (13-)
a″	1458	1463	210-7 (81+)	210-8 (14+)		
	1432	1432	014-7 (96+)			
	1305	1303	222-6 (47-)	221-6 (26+)		
	1276	1276	221-6 (39+)	422-6 (28-)	222-6 (7+)	
	1204	1208	422-6 (27-)	221-4 (17+)	210-8 (17+)	222-6 (12-)
		1079	422-6 (33-)	222-6 (17-)	422-4 (14-)	222-4 (11-)
	959	958	014-8 (94+)			
	916	913	210-8 (31-)	422-4 (28+)	221-6 (25-)	222-4 (17+)
	788	781	422-4 (39-)	221-4 (31+)	210-8 (20-)	
	724	730	222-4 (42-)	221-4 (37+)	422-4 (11+)	
	220	231	2210-T(92+)			
		163	0142-T(87+)			
		132	2221-T(64+)	1422-T(14-)	0142-T(10+)	
		99	4222-T(73+)			
		53	1422-T(76-)	2221-T(17-)		

Calculated frequencies higher than 2000 cm^{-1}

2962 2962 2954 2953 2944 2909 2906 2900 2880 2873
2865 2857

Reference

[1] IR.R. M. Ohta, Y. Ogawa, H. Matsuura, I. Harada, and T. Shimanouchi, Bull. Chem. Soc. Jpn., **50**, 380 (1977).

No. 94
Molecule: 142221-TGT $CH_3SCH_2CH_2CH_2CH_3$ (trans-gauche-trans form)
Symmetry C_1 Symmetry number $\sigma = 1$

Sym. species	Observed frequency cm^{-1}	Calculated frequency cm^{-1}	Assignment (P.E.D. %)			
a	1476*(s)	1486	222-2 (39+)	221-2 (36-)	210-4 (12-)	
	1464*	1465	222-2 (40+)	210-4 (20+)	221-2 (18+)	
	1458*	1463	210-7 (79+)	210-8 (14+)		
	1452*	1453	210-4 (44-)	221-2 (26+)	422-2 (8+)	
	1445*	1448	014-4 (29-)	422-2 (19-)	221-2 (14+)	222-2 (11+)
	1445*	1438	014-4 (63-)	422-2 (13+)		
	1432*	1432	014-7 (96+)			
	1378*	1391	422-2 (35+)	222-5 (32+)	221-5 (10-)	
	1378*	1379	210-2 (105+)			
	1324*	1324	014-2 (68+)	221-5 (24-)		
	1324*	1316	221-5 (47+)	014-2 (33+)		
	1305*	1305	222-6 (43-)	221-6 (20+)	422-6 (12-)	
	1276*	1272	221-6 (47-)	422-6 (16-)	210-8 (6+)	210-7 (5-)
	1204*	1204	422-5 (17-)	221-4 (15-)	422-6 (14-)	210-8 (14-)
	1169	1172	422-5 (27-)	222-5 (24+)	422-6 (21+)	4222-S(16-)
	1101*	1109	4222-S(23+)	2221-S(23-)	422-5 (9+)	221-4 (7-)
	1082*	1082	422-6 (28-)	210-5 (14+)	422-4 (10-)	222-6 (9+)
	1053*	1045	2210-S(40-)	2221-S(15+)	422-5 (8+)	222-6 (6-)
	1001	1006	2210-S(36+)	4222-S(34-)	422-5 (5+)	
	968*	966	014-5 (91-)			
	959*	958	014-8 (94-)			
	916*	921	422-4 (31-)	210-5 (31-)	221-5 (10+)	
	872	874	222-4 (33+)	210-8 (32-)	221-6 (20-)	
	813	804	422-4 (40+)	2221-S(31-)		
	748*	743	221-4 (59+)	222-4 (17-)	210-8 (16-)	
	725	726	0142-S(95+)			
	672	672	1422-S(74-)	222-4 (13-)		
	489	498	222-D (23-)	221-D (18-)	422-D (12+)	1422-S(7+)
	295	295	221-D (55-)	422-D (23-)	4222-S(10-)	
	267	268	222-D (39-)	142-B (33-)	221-D (12+)	
		235	2210-T(64+)	142-B (26-)		
		208	422-D (33-)	142-B (31+)	2210-T(26+)	2221-T(11-)
		158	0142-T(96+)			
		97	4222-T(57+)	2221-T(28+)		
		79	2221-T(45+)	422-D (31-)	4222-T(10-)	
		48	1422-T(91+)			

Calculated frequencies higher than 2000 cm^{-1}
2962 2962 2954 2953 2944 2909 2906 2900 2880 2873
2865 2857

* Weight of the observed frequency is zero.

Reference

[1] IR.R. M. Ohta, Y. Ogawa, H. Matsuura, I. Harada, and T. Shimanouchi, Bull. Chem. Soc. Jpn., **50**, 380 (1977).

No. 95

Molecule: 142221-GTT $CH_3SCH_2CH_2CH_2CH_3$ (gauche-trans-trans form)

Symmetry C_1 Symmetry number σ = 1

Sym. species	Observed frequency cm^{-1}	Calculated frequency cm^{-1}	Assignment (P.E.D. %)			
a	1476*(s)	1487	222-2 (46-)	221-2 (33+)	210-4 (11+)	
	1464*	1465	222-2 (46+)	221-2 (22+)	210-4 (21+)	
	1458*	1463	210-7 (81+)	210-8 (14+)		
	1452*	1453	210-4 (52+)	221-2 (38-)		
	1445*	1442	014-4 (96+)			
	1429	1432	014-7 (96+)			
	1424*	1412	422-2 (87+)			
	1378*	1379	210-2 (105+)			
	1354*	1355	221-5 (52+)	222-5 (34-)	2221-S(16-)	
	1324*	1322	014-2 (101+)			
	1305*	1302	222-6 (45-)	221-6 (29+)		
	1296*	1292	222-5 (32+)	422-5 (32-)	221-5 (25+)	
	1276*	1275	221-6 (36+)	422-6 (30-)	222-6 (9+)	
	1227*	1226	422-5 (58+)	222-5 (28+)		
	1204*	1208	422-6 (28-)	221-4 (17+)	210-8 (17+)	222-6 (12-)
	1101*	1098	210-5 (24+)	2221-S(21-)	221-5 (10-)	222-5 (9-)
	1082	1075	422-6 (30+)	222-6 (20+)	422-4 (12+)	222-4 (11+)
	1053*	1055	2221-S(29-)	2210-S(28+)	4222-S(28+)	
	1012*	1013	2210-S(50+)	4222-S(43-)		
	968*	968	014-5 (90+)			
	959*	958	014-8 (95+)			
	903	902	210-8 (28-)	221-6 (21-)	422-4 (20+)	222-4 (19+)
	897*	898	210-5 (37-)	2221-S(27-)	221-5 (9+)	
	775	770	422-4 (36-)	221-4 (32+)	210-8 (16-)	
	753	756	1422-S(52+)	0142-S(21-)		
	724*	728	222-4 (41-)	221-4 (27+)	422-4 (20+)	
	697	699	0142-S(78-)	1422-S(21-)		
	406	405	221-D (61+)	422-D (25-)		
	353	351	142-B (36-)	222-D (22+)	422-D (15+)	1422-S(10+)
	277	267	142-B (73+)	222-D (14+)	422-4 (10+)	
	220*	229	2210-T(91+)			
		171	0142-T(51+)	222-D (19-)	422-D (18+)	221-D (14+)
		140	0142-T(48+)	422-D (23-)	222-D (16+)	
		123	2221-T(64-)	422-D (10+)		
		89	4222-T(81-)			
		55	1422-T(79-)	2221-T(14-)		

Calculated frequencies higher than 2000 cm^{-1}

2962 2962 2954 2953 2943 2909 2905 2900 2880 2873
2865 2857

* Weight of the observed frequency is zero.

Reference

[1] IR.R. M. Ohta, Y. Ogawa, H. Matsuura, I. Harada, and T. Shimanouchi, Bull. Chem. Soc. Jpn., **50**, 380 (1977).

No. 96

Molecule: 142221-GGT $CH_3SCH_2CH_2CH_2CH_3$ (gauche-gauche-trans form)

Symmetry C_1 Symmetry number $\sigma = 1$

Sym. species	Observed frequency cm^{-1}	Calculated frequency cm^{-1}	Assignment (P.E.D. %)			
a	1476*(s)	1485	221-2 (39-)	222-2 (37+)	210-4 (13-)	
	1464*	1463	222-2 (39+)	210-7 (19+)	210-4 (19+)	221-2 (10+)
	1458*	1463	210-7 (62+)	222-2 (12-)	210-8 (11+)	
	1452*	1452	210-4 (45-)	221-2 (40+)		
	1445*	1442	014-4 (95+)			
	1432*	1438	422-2 (38+)	422-5 (18-)	222-5 (18-)	
	1432*	1432	014-7 (96+)			
	1378*	1384	422-2 (42+)	222-5 (26+)	221-5 (10-)	
	1378*	1379	210-2 (98+)			
	1324*	1322	014-2 (90+)	221-5 (10+)		
	1305*	1312	221-5 (58+)	014-2 (13-)		
	1305*	1301	222-6 (38-)	221-6 (25+)	422-6 (13-)	
	1276*	1262	221-6 (42-)	422-6 (19-)	210-8 (7+)	222-6 (7-)
	1193	1198	422-5 (25-)	222-6 (15+)	221-4 (12-)	210-8 (11-)
	1169	1168	422-6 (29-)	222-5 (22-)	422-5 (18+)	4222-S(10+)
	1101*	1105	4222-S(24-)	2221-S(17+)	221-4 (11+)	222-4 (9+)
	1082*	1079	422-6 (23-)	210-5 (18+)	222-6 (9+)	2210-S(8-)
	1053*	1047	2210-S(40-)	2221-S(16+)	422-5 (8+)	4222-S(6-)
	1001*	1004	4222-S(37-)	2210-S(37+)		
	968*	968	014-5 (89+)			
	959*	958	014-8 (95+)			
	916*	912	210-5 (31-)	422-4 (26-)	2221-S(10-)	221-5 (8+)
	878	881	222-4 (32+)	210-8 (30-)	221-6 (16-)	
	788*	793	422-4 (50+)	2221-S(24-)		
	748	745	221-4 (52+)	222-4 (16-)	210-8 (15-)	
	725	723	0142-S(83+)	1422-S(10-)		
	654	658	1422-S(76-)	0142-S(18-)		
	481	475	222-D (28-)	221-D (18-)	422-D (18+)	422-4 (9-)
	333	326	142-B (81+)	422-D (23-)		
	295	296	221-D (63+)	222-D (16-)	422-D (13+)	
		234	2210-T(82+)			
		190	142-B (31-)	422-D (25-)	222-D (20-)	2210-T(11+)
		157	0142-T(95+)			
		99	4222-T(58-)	222-D (12-)	1422-T(10+)	
		89	2221-T(71+)	422-D (13-)		
		43	1422-T(78+)	4222-T(12+)		

Calculated frequencies higher than 2000 cm^{-1}

2962 2962 2954 2953 2943 2909 2905 2900 2880 2873
2865 2857

* Weight of the observed frequency is zero.

Reference

[1] IR.R. M. Ohta, Y. Ogawa, H. Matsuura, I. Harada, and T. Shimanouchi, Bull. Chem. Soc. Jpn., **50**, 380 (1977).

No. 97

Molecule: 142241-TTT $CH_3SCH_2CH_2SCH_3$ (trans-trans-trans form)

Symmetry C_{2h} Symmetry number $\sigma = 2$

Sym. species	Observed frequency cm^{-1}	Calculated frequency cm^{-1}	Assignment (P.E.D. %)			
a_g	1439*	1446	410-4 (33+)	014-4 (33+)	224-2 (13+)	422-2 (13+)
	1428*	1431	224-2 (30+)	422-2 (30+)	014-4 (15-)	410-4 (15-)
	1322*	1324	410-2 (47+)	014-2 (47+)		
	1270*	1271	422-5 (47+)	224-5 (47-)	4224-S(17+)	
	1045*	1046	4224-S(63-)	224-2 (5+)	422-2 (5+)	
	960*	965	014-5 (45+)	410-5 (45+)		
	765*	759	1422-S(40-)	2241-S(40-)	422-D (16+)	224-D (16+)
	725*	722	2410-S(50+)	0142-S(50+)		
	268	272	224-D (33+)	422-D (33+)	2241-S(8+)	
	230*	225	241-B (48+)	142-B (48+)		
a_u	1432*	1432	410-7 (48+)	014-7 (48+)		
	1134*	1146	224-6 (49+)	422-6 (49+)		
	960*	957	014-8 (48+)	410-8 (48+)		
		754	224-4 (45-)	422-4 (45+)	4224-T(11-)	
		171	0142-T(38+)	2410-T(38+)	4224-T(20-)	
		118	4224-T(64+)	2410-T(12+)	0142-T(12+)	
		42	2241-T(48+)	1422-T(48+)		
b_g	1428*	1432	014-7 (48+)	410-7 (48-)		
	1284*	1288	422-6 (40-)	224-6 (40+)		
	976	987	422-4 (39+)	224-4 (39+)		
	960*	955	410-8 (44+)	014-8 (44-)		
		159	2410-T(49+)	0142-T(49-)		
		95	1422-T(49-)	2241-T(49+)		
b_u	1436*	1444	014-4 (40-)	410-4 (40+)		
	1425*	1429	224-2 (38-)	422-2 (38+)		
	1323*	1321	014-2 (51+)	410-2 (51-)		
	1206*	1193	224-5 (54+)	422-5 (54+)		
	960*	966	410-5 (46-)	014-5 (46+)		
	736*	743	0142-S(28+)	2410-S(28-)	2241-S(20+)	1422-S(20-)
	684*	695	2241-S(28-)	1422-S(28+)	2410-S(24-)	0142-S(24+)
	395	396	142-B (33-)	241-B (33+)	422-D (11-)	224-D (11+)
		107	422-D (52-)	224-D (52+)	142-B (23+)	241-B (23-)

Calculated frequencies higher than 2000 cm^{-1}

2954 2954 2953 2953 2948 2939 2910 2901 2857 2857

* Weight of the observed frequency is zero.

Reference

[1] IR.R. Y. Ogawa, M. Ohta, M. Sakakibara, H. Matsuura, I. Harada, and T. Shimanouchi, Bull. Chem. Soc. Jpn., **50**, 650 (1977).

No. 98
Molecule: 142241-TTG $CH_3SCH_2CH_2SCH_3$ (trans-trans-gauche form)
Symmetry C_1 Symmetry number $\sigma = 1$

Sym. species	Observed frequency cm^{-1}	Calculated frequency cm^{-1}	Assignment (P.E.D. %)			
a	1439*	1445	014-4 (74+)	422-2 (20+)		
	1436*	1442	410-4 (96+)			
	1432*	1432	410-7 (95+)			
	1425*	1432	014-7 (96+)			
	1425*	1430	422-2 (67+)	014-4 (22-)		
	1415*	1419	224-2 (88-)			
	1323*	1324	014-2 (74+)	410-2 (23-)		
	1322*	1321	410-2 (79+)	014-2 (24+)		
	1284*	1285	224-6 (41-)	422-6 (39+)		
	1272	1274	224-5 (48-)	422-5 (44+)	4224-S(18+)	
	1190	1194	422-5 (57+)	224-5 (50+)		
	1134*	1147	422-6 (51+)	224-6 (48+)		
	1036	1038	4224-S(67-)	422-2 (5+)		
	976	977	410-5 (37+)	422-4 (23+)	224-4 (21+)	
	970*	965	014-5 (90+)			
	970*	962	410-5 (43+)	014-8 (30+)	422-4 (11-)	
	960*	957	410-8 (84+)	014-8 (11-)		
	960*	953	014-8 (50+)	422-4 (15+)	224-4 (11+)	410-5 (11-)
	775*	764	2241-S(48-)	1422-S(18-)	2410-S(16+)	422-D (14+)
	736*	746	224-4 (43-)	422-4 (31+)	1422-S(12-)	4224-T(10-)
	735	737	1422-S(39-)	0142-S(35+)		
	714	716	0142-S(45+)	2410-S(42+)	1422-S(14+)	
	687	688	2410-S(41+)	2241-S(38+)	0142-S(16-)	
	348	351	142-B (41+)	224-D (36-)	241-B (36+)	
	300	308	241-B (38+)	142-B (20-)	422-D (19-)	
	245*	243	241-B (46+)	422-D (19+)	224-D (15+)	
		165	0142-T(52+)	2410-T(28-)		
		161	2410-T(48+)	0142-T(39+)		
		129	422-D (38+)	224-D (28-)	142-B (26-)	2410-T(22+)
		103	4224-T(64+)	0142-T(8+)		
		88	1422-T(44-)	2241-T(39+)		
		44	2241-T(48+)	1422-T(48+)		

Calculated frequencies higher than 2000 cm^{-1}

2954 2954 2953 2953 2947 2939 2909 2901 2857 2857

* Weight of the observed frequency is zero.

Reference

[1] IR.R. Y. Ogawa, M. Ohta, M. Sakakibara, H. Matsuura, I. Harada, and T. Shimanouchi, Bull. Chem. Soc. Jpn., **50**, 650 (1977).

No. 99
Molecule: 142241-TGG $CH_3SCH_2CH_2SCH_3$ (trans-gauche-gauche form)
Symmetry C_1 Symmetry number $\sigma = 1$

Sym. species	Observed frequency cm^{-1}	Calculated frequency cm^{-1}	Assignment (P.E.D. %)			
a	1439*	1446	014-4 (59+)	422-2 (28+)		
	1436*	1442	410-4 (96+)			
	1432*	1434	422-2 (40+)	014-4 (35-)	224-2 (17+)	
	1432*	1432	410-7 (93+)			
	1432*	1432	014-7 (94+)			
	1425*	1422	224-2 (57+)	224-5 (14+)	422-2 (11-)	
	1323*	1330	014-2 (27-)	422-5 (21+)	410-2 (17-)	224-5 (17+)
	1323*	1322	410-2 (57+)	014-2 (45-)		
	1322*	1314	014-2 (30+)	410-2 (29+)	224-5 (16+)	422-5 (12+)
	1272*	1284	224-6 (37+)	422-6 (35+)		
	1181	1179	422-5 (46+)	224-5 (45-)	4224-S(29+)	
	1134*	1141	224-6 (49+)	422-6 (48-)		
	1024*	1021	4224-S(64+)	422-4 (6+)	224-4 (4-)	
	976*	972	410-5 (71+)			
	970*	966	014-5 (85+)			
	960*	958	014-8 (74+)	410-8 (15+)		
	960*	958	410-8 (79-)	014-8 (15+)		
		936	422-4 (38-)	224-4 (20+)	410-5 (14-)	
	845*	860	224-4 (42+)	422-4 (21+)	422-D (9+)	
	725	726	0142-S(94+)			
	725	723	2410-S(87+)	2241-S(11-)		
	661	672	1422-S(44+)	2241-S(19-)	224-4 (14+)	
	650	646	2241-S(59-)	1422-S(30-)		
	435	438	224-D (28+)	422-D (21-)	1422-S(10-)	142-B (9-)
	311	315	241-B (91-)	224-4 (12+)	224-D (12+)	422-D (10+)
	250	244	142-B (79+)	224-D (16+)		
		195	4224-T(35-)	241-B (21+)	422-D (19+)	0142-T(14+)
		156	2410-T(95+)			
		152	0142-T(84+)			
		93	422-D (54-)	224-D (36-)	4224-T(29-)	
		51	1422-T(64+)	2241-T(24+)		
		41	2241-T(62+)	1422-T(28-)		

Calculated frequencies higher than 2000 cm^{-1}
2954 2954 2953 2953 2945 2941 2907 2903 2857 2857
* Weight of the observed frequency is zero.

Reference

[1] IR.R. Y. Ogawa, M. Ohta, M. Sakakibara, H. Matsuura, I. Harada, and T. Shimanouchi, Bull. Chem. Soc. Jpn., **50**, 650 (1977).

No. 100

Molecule: 142241-GTG′ $CH_3SCH_2CH_2SCH_3$ (gauche-trans-gauche′ form)

Symmetry C_i Symmetry number $\sigma = 1$

Sym. species	Observed frequency cm^{-1}	Calculated frequency cm^{-1}	Assignment (P.E.D. %)			
a_g	1439	1442	410-4 (48+)	014-4 (48+)		
	1428	1432	014-7 (49+)	410-7 (49-)		
	1415	1415	224-2 (45+)	422-2 (45+)		
	1322	1323	410-2 (50+)	014-2 (50+)		
	1284	1284	422-6 (34+)	224-6 (34-)	422-5 (9+)	
	1270	1276	422-5 (38+)	224-5 (38-)	4224-S(16+)	
	1024	1030	4224-S(71+)			
	970	968	410-5 (46+)	014-5 (46-)		
	960	958	014-8 (47-)	410-8 (47+)		
		938	224-4 (38+)	422-4 (38+)		
	765	764	1422-S(32-)	2241-S(32-)	422-D (14+)	224-D (14+)
	700	697	0142-S(40+)	2410-S(40+)	1422-S(11+)	2241-S(11+)
	339	340	142-B (32+)	241-B (32+)	422-D (16-)	224-D (16-)
	230	221	241-B (25+)	142-B (25+)	422-D (13+)	224-D (13+)
		154	0142-T(48+)	2410-T(48-)		
		85	2241-T(46-)	1422-T(46+)		
a_u	1436	1442	014-4 (48-)	410-4 (48+)		
	1432	1432	410-7 (48+)	014-7 (48+)		
	1425	1424	422-2 (46+)	224-2 (46-)		
	1323	1321	014-2 (52-)	410-2 (52+)		
	1206	1196	224-5 (53+)	422-5 (53+)		
	1134	1147	224-6 (50+)	422-6 (50+)		
	960	972	014-5 (37+)	410-5 (37+)		
	960	957	410-8 (48+)	014-8 (48+)		
	736	746	422-4 (22+)	224-4 (22-)	2241-S(18-)	1422-S(18+)
	727	735	0142-S(21+)	2410-S(21-)	224-4 (18-)	422-4 (18+)
	684	689	2410-S(25-)	0142-S(25+)	2241-S(23-)	1422-S(23+)
	309	309	241-B (58+)	142-B (58-)	224-4 (13+)	422-4 (13-)
		209	224-D (37-)	422-D (37+)	0142-T(11+)	2410-T(11+)
		144	2410-T(39-)	0142-T(39-)	224-D (12-)	422-D (12+)
		90	4224-T(71-)			
		41	1422-T(46+)	2241-T(46+)		

Calculated frequencies higher than 2000 cm^{-1}

2954 2954 2953 2953 2946 2939 2909 2900 2857 2857

Reference

[1] IR.R. Y. Ogawa, M. Ohta, M. Sakakibara, H. Matsuura, I. Harada, and T. Shimanouchi, Bull. Chem. Soc. Jpn., **50**, 650 (1977).

No. 101
Molecule: 142241-GGG $CH_3SCH_2CH_2SCH_3$ (gauche-gauche-gauche form)
Symmetry C_2 **Symmetry number** $\sigma = 2$

Sym. species	Observed frequency cm^{-1}	Calculated frequency cm^{-1}	Assignment (P.E.D. %)			
a	1439*	1442	410-4 (48+)	014-4 (48+)		
	1432*	1432	410-7 (48+)	014-7 (48+)		
	1432*	1427	422-2 (45+)	224-2 (45+)		
	1322*	1322	014-2 (52+)	410-2 (52+)		
	1284*	1283	422-6 (36+)	224-6 (36+)		
	1181	1182	224-5 (45-)	422-5 (45-)	4224-S(30-)	
	1010	1008	4224-S(71+)			
	976*	973	014-5 (39-)	410-5 (39-)		
	960*	957	410-8 (48+)	014-8 (48+)		
	915	921	422-4 (34+)	224-4 (34-)	410-5 (8+)	
	725*	722	2410-S(47+)	0142-S(47+)		
	635	637	2241-S(46+)	1422-S(46+)		
	330	327	142-B (41-)	241-B (41-)	224-D (15+)	422-D (15+)
		163	0142-T(32+)	2410-T(32+)	4224-T(18+)	
		151	4224-T(18+)	422-D (17-)	224-D (17-)	2410-T(15-)
		102	422-D (45-)	224-D (45-)	4224-T(19-)	
		40	1422-T(38+)	2241-T(38+)	4224-T(22+)	
b	1436*	1442	014-4 (48+)	410-4 (48-)		
	1432*	1432	014-7 (48+)	410-7 (48-)		
	1425*	1422	224-2 (32+)	422-2 (32-)	224-5 (13+)	422-5 (13+)
	1323*	1328	410-2 (25-)	014-2 (25+)	422-5 (16+)	224-5 (16+)
	1323*	1314	014-2 (27-)	410-2 (27+)	422-5 (16+)	224-5 (16+)
	1134*	1143	224-6 (48+)	422-6 (48-)		
	970*	967	410-5 (46+)	014-5 (46-)		
	960*	958	014-8 (48-)	410-8 (48+)		
	845	848	422-4 (32+)	224-4 (32+)	422-D (9+)	
	725*	723	0142-S(42+)	2410-S(42-)		
	661*	667	1422-S(31+)	2241-S(31-)	2410-S(11-)	0142-S(11+)
	418	413	422-D (34-)	224-D (34+)	422-4 (9+)	
	295	296	241-B (61+)	142-B (61-)		
		154	0142-T(49+)	2410-T(49-)		
		47	2241-T(48-)	1422-T(48+)		

Calculated frequencies higher than 2000 cm^{-1}

2954 2954 2953 2953 2944 2941 2906 2903 2857 2857

* Weight of the observed frequency is zero.

Reference

[1] IR.R. Y. Ogawa, M. Ohta, M. Sakakibara, H. Matsuura, I. Harada, and T. Shimanouchi, Bull. Chem. Soc. Jpn., **50**, 650 (1977).

No. 102
Molecule: (422) $(SCH_2CH_2)_n$
Symmetry[a] C_{2h}

Sym. species	Observed frequency cm^{-1}	Calculated frequency cm^{-1}	Assignment (P.E.D. %)			
a_g	1426(s)	1414	224–2 (90+)			
	1276(s)	1277	224–6 (89+)			
	1276(s)	1274	224–5 (98+)	4224–S(19–)		
	1031(s)	1026	4224–S(75–)			
	900(s)	900	224–4 (115+)			
	731(s)	721	2242–S(86–)	224–D (38+)		
	338(s)	349	242–B (81–)	224–D (33+)	224–4 (10+)	
	180(s)	185	242–B (39+)	224–D (28+)	2242–S(16+)	2242–T(13–)
a_u	1423(s)	1421	224–2 (93+)			
	1190(s)	1193	224–5 (98+)			
	1143(s)	1150	224–6 (86+)			
	723(s)	731	224–4 (56+)	2242–S(19–)	4224–T(13+)	
	672(s)	682	2242–S(77+)	224–4 (26+)		
		307	242–B (150+)	224–4 (58–)		
	176(s)	179	224–D (110+)			
b_g	1426(s)	1416	224–2 (89+)			
	1297(s)	1288	224–6 (91+)			
	1276(s)	1278	224–5 (104+)	4224–S(21–)		
	1031(s)	1027	4224–S(75–)			
	998(s)	985	224–4 (92+)			
	760(s)	767	2242–S(88–)	224–D (37+)		
	320(s)	308	224–D (61+)	2242–S(20+)		
		101	2242–T(98+)			
b_u	1423(s)	1425	224–2 (91+)			
	1183(s)	1195	224–5 (98+)	224–2 (10–)		
	1143(s)	1146	224–6 (86+)			
	749(s)	760	224–4 (63+)	2242–S(24–)	224–6 (13+)	
	723(s)	732	2242–S(75+)	224–4 (18+)		
	251(s)	250	224–D (107+)			
	139(s)	125	4224–T(80+)	224–4 (16–)		

[a] The point group given is that to which the symmetry of the molecular chain is isomorphous. The internal-rotation angles of τ(C-C)=180° and τ(C-S)=±79.3° were used in the calculation.

Calculated frequencies higher than 2000 cm^{-1}

2948 2945 2939 2939 2909 2908 2900 2900

References

[1] R. A. C. Angood and J. L. Koenig, J. Macromol. Sci.-Phys., **B3**, 321 (1969).

[2] IR.R. M. Yokoyama, H. Ochi, A. M. Ueda, and H. Tadokoro, J. Macromol. Sci.-Phys., **B7**, 465 (1973).

No. 103
Molecule: (42'2') $(SCD_2CD_2)_n$
Symmetry[a] C_{2h}

Sym. species	Observed frequency cm^{-1}	Calculated frequency cm^{-1}	Assignment (P.E.D. %)			
a_g	1125(s)	1126	4224-S(74-)	224-5 (26+)	224-2 (24-)	
	1031(s)	1034	224-5 (53+)	224-2 (47+)	2242-S(12+)	
	906(s)	929	224-6 (87+)	224-4 (12+)		
	830(s)	834	224-5 (37-)	224-2 (30+)	4224-S(17-)	224-D (10+)
	703(s)	718	224-4 (107+)	242-B (12-)		
	657(s)	662	2242-S(69-)	224-D (27+)		
	328(s)	331	242-B (66-)	224-D (40+)		
		159	242-B (48+)	224-D (22+)	2242-T(14-)	2242-S(14+)
a_u	1056(s)	1055	224-2 (75+)	224-5 (13+)	2242-S(10+)	
	921(s)	922	224-5 (81+)	224-2 (26-)		
	843(s)	832	224-6 (81+)			
	654(s)	642	2242-S(78+)			
	520(s)	511	224-4 (83+)	4224-T(14+)	224-6 (13+)	
	297(s)	290	242-B (148+)	224-4 (55-)	224-6 (10-)	
		166	224-D (109+)			
b_g	1125(s)	1127	4224-S(74-)	224-5 (27+)	224-2 (22-)	
	1031(s)	1038	224-5 (52+)	224-2 (48+)	2242-S(12+)	
		958	224-6 (67+)	224-4 (27+)		
	830(s)	836	224-5 (35-)	224-2 (30+)	4224-S(15-)	224-D (12+)
		788	224-4 (62+)	224-6 (29-)		
	703(s)	710	2242-S(65-)	224-D (25+)		
	318(s)	305	224-D (62-)	2242-S(19-)		
		83	2242-T(99+)			
b_u	1055(s)	1062	224-2 (71+)	224-5 (14+)	2242-S(11+)	
	919(s)	922	224-5 (80+)	224-2 (29-)		
	843(s)	829	224-6 (78+)			
	690(s)	689	2242-S(81+)			
	553(s)	552	224-4 (81+)	224-6 (18+)		
	238(s)	238	224-D (106+)			
	126(s)	114	4224-T(82+)	224-4 (13-)		

[a] The point group given is that to which the symmetry of the molecular chain is isomorphous. The internal-rotation angles of τ(C-C)=180° and τ(C-S)=±79.3° were used in the calculation.

Calculated frequencies higher than 2000 cm^{-1}

2202 2194 2179 2179 2143 2142 2118 2118

Reference

[1] IR.R. M. Yokoyama, H. Ochi, A. M. Ueda, and H. Tadokoro, J. Macromol. Sci.-Phys., **B7**, 465 (1973).

No. 104
Molecule: 132241-TTT $CH_3OCH_2CH_2SCH_3$ (trans-trans-trans form)
Symmetry C_s Symmetry number $\sigma = 1$

Sym. species	Observed frequency cm^{-1}	Calculated frequency cm^{-1}	Assignment (P.E.D. %)			
a′	1480*	1484	322-2 (96+)			
	1465*	1468	013-4 (83+)	013-5 (16+)		
	1460*	1461	013-2 (103+)			
	1449*	1445	410-4 (74+)	224-2 (19+)		
	1432*	1430	224-2 (66+)	410-4 (22-)		
	1382*	1378	322-5 (85+)			
	1325*	1322	410-2 (101+)			
	1245*	1237	224-5 (98+)			
	1196*	1200	013-5 (59+)	1322-S(19-)	322-5 (10+)	013-4 (10-)
	1122*	1119	0132-S(49-)	3224-S(19-)	1322-S(11+)	
	1055*	1063	3224-S(38-)	0132-S(24+)	1322-S(9-)	
	968*	970	410-5 (43+)	1322-S(33-)	0132-S(11-)	
	964*	961	410-5 (48+)	1322-S(35+)	0132-S(10+)	
	758	763	2241-S(76-)			
	720	721	2410-S(98+)			
	468	473	132-B (52-)	241-B (16+)	224-D (11+)	322-D (11-)
	340	343	322-D (30+)	224-D (17+)	2241-S(17+)	132-B (9-)
	265	267	241-B (58+)	132-B (22+)		
		119	224-D (78+)	322-D (44-)	241-B (32-)	
a″	1455*	1454	013-7 (86+)	013-8 (16+)		
	1432*	1432	410-7 (96+)			
	1281*	1282	322-6 (71+)	224-6 (16-)		
	1218*	1221	224-6 (62+)	322-4 (16+)		
	1156*	1153	013-8 (77+)	013-7 (11-)		
	980*	984	322-4 (54+)	224-4 (33+)	224-6 (13-)	
	959*	956	410-8 (91+)			
	814*	808	224-4 (60+)	322-4 (24-)	322-6 (15+)	
	228*	220	0132-T(83-)	3224-T(12+)		
		164	2410-T(79+)			
		137	1322-T(56-)	2410-T(17-)	3224-T(10-)	
		106	3224-T(62+)	1322-T(14-)	2241-T(10+)	
		57	2241-T(79+)	1322-T(15+)		

Calculated frequencies higher than 2000 cm^{-1}
2989 2988 2964 2954 2953 2942 2906 2865 2857 2820

* Weight of the observed frequency is zero.

Reference

[1] IR.R. Y. Ogawa, M. Ohta, M. Sakakibara, H. Matsuura, I. Harada, and T. Shimanouchi, Bull. Chem. Soc. Jpn., **50**, 650 (1977).

No. 105
Molecule: 132241-TTG $CH_3OCH_2CH_2SCH_3$ (trans-trans-gauche form)
Symmetry C_1 Symmetry number $\sigma = 1$

Sym. species	Observed frequency cm^{-1}	Calculated frequency cm^{-1}	Assignment (P.E.D. %)			
a	1480	1484	322-2 (96+)			
	1465	1468	013-4 (83+)	013-5 (16+)		
	1460	1461	013-2 (103+)			
	1455	1454	013-7 (86+)	013-8 (16+)		
	1449	1442	410-4 (96+)			
	1432	1432	410-7 (96+)			
	1420	1419	224-2 (88+)			
	1382	1379	322-5 (85+)			
	1325	1322	410-2 (103+)			
	1281	1280	322-6 (71+)	224-6 (16-)		
	1245	1241	224-5 (95+)			
	1218	1222	224-6 (62+)	322-4 (15+)		
	1196	1199	013-5 (59+)	1322-S(19-)	322-5 (10+)	013-4 (10-)
	1156	1153	013-8 (77+)	013-7 (12-)		
	1113	1119	0132-S(52-)	3224-S(17-)	1322-S(12+)	
	1055	1055	3224-S(45-)	0132-S(23+)	1322-S(7-)	
	980	975	410-5 (36+)	322-4 (35+)	224-4 (18+)	
	964	966	1322-S(54-)	0132-S(16-)	322-D (8+)	
	959	962	410-5 (49+)	322-4 (23-)	1322-S(11+)	
	945	957	410-8 (87+)			
	792	791	224-4 (63+)	322-4 (15-)	322-6 (11+)	
	765	768	2241-S(59+)	2410-S(15-)		
	703	703	2410-S(88+)	2241-S(13+)		
	441	440	132-B (69-)	224-D (19+)		
	363	367	241-B (29+)	322-D (21-)	2241-S(14-)	224-D (13-)
	281	275	241-B (82+)	224-4 (12-)	322-D (11+)	
	218	217	0132-T(86-)			
		174	2410-T(45-)	224-D (27-)	322-D (22+)	132-B (10-)
		141	2410-T(52+)	224-D (23-)	322-D (15+)	1322-T(11-)
		128	1322-T(58+)	224-D (17-)		
		96	3224-T(73-)			
		59	2241-T(81+)	1322-T(12+)		

Calculated frequencies higher than 2000 cm^{-1}

2989 2988 2964 2954 2953 2942 2905 2865 2857 2820

Reference

[1] IR.R. Y. Ogawa, M. Ohta, M. Sakakibara, H. Matsuura, I. Harada, and T. Shimanouchi, Bull. Chem. Soc. Jpn., **50**, 650 (1977).

No. 106
Molecule: 132241-TGT $CH_3OCH_2CH_2SCH_3$ (trans-gauche-trans form)
Symmetry C_1 Symmetry number $\sigma = 1$

Sym. species	Observed frequency cm^{-1}	Calculated frequency cm^{-1}	Assignment (P.E.D. %)			
a	1480*	1483	322-2 (88+)			
	1465*	1468	013-4 (83+)	013-5 (16+)		
	1460*	1461	013-2 (103+)			
	1455*	1454	013-7 (86+)	013-8 (16+)		
	1449*	1444	410-4 (83+)	224-2 (10+)		
	1432*	1432	410-7 (96+)			
	1420*	1426	224-2 (68+)	410-4 (13-)		
	1405*	1401	322-5 (81+)	3224-S(10+)		
	1325*	1322	410-2 (101+)			
	1290*	1292	322-6 (54+)	224-6 (19+)		
	1245*	1248	224-5 (81+)			
	1218*	1219	013-5 (35+)	1322-S(21-)	224-6 (17+)	322-6 (11-)
	1180*	1178	224-6 (31-)	013-5 (23+)	013-8 (19-)	
	1135*	1148	013-8 (60+)	224-6 (13-)	322-6 (11+)	
	1122*	1120	0132-S(44-)	3224-S(19-)	1322-S(17+)	013-5 (10+)
	1055*	1058	3224-S(36+)	0132-S(34-)	322-4 (14+)	
	1012	1007	224-4 (24-)	322-4 (22+)	1322-S(11+)	3224-S(11-)
	968	972	410-5 (52+)	1322-S(11+)	322-4 (7-)	322-D (6-)
	964*	959	410-8 (45+)	410-5 (26+)		
	959*	955	410-8 (47-)	1322-S(14-)	410-5 (13+)	
	814	804	224-4 (46+)	1322-S(34+)		
	729*	726	2410-S(93+)			
	685	675	2241-S(77-)			
	520	528	322-D (26+)	132-B (23+)	224-D (9-)	2241-S(6-)
	335*	321	132-B (60+)	224-D (18+)	322-D (13-)	
	290	279	322-D (33-)	241-B (26-)	3224-T(12+)	
	228*	228	241-B (51+)	0132-T(32-)	224-D (21-)	3224-T(13+)
		206	0132-T(56+)	224-D (20-)	241-B (17+)	1322-T(14-)
		158	2410-T(96+)			
		111	3224-T(49+)	1322-T(33+)		
		85	1322-T(42-)	224-D (30+)	3224-T(17+)	
		49	2241-T(92+)			

Calculated frequencies higher than 2000 cm^{-1}

2989 2988 2964 2954 2953 2943 2905 2865 2857 2820

* Weight of the observed frequency is zero.

Reference

[1] IR.R. Y. Ogawa, M. Ohta, M. Sakakibara, H. Matsuura, I. Harada, and T. Shimanouchi, Bull. Chem. Soc. Jpn., **50**, 650 (1977).

No. 107
Molecule: 132241-TGG $CH_3OCH_2CH_2SCH_3$ (trans-gauche-gauche form)
Symmetry C_1 Symmetry number $\sigma = 1$

Sym. species	Observed frequency cm^{-1}	Calculated frequency cm^{-1}	Assignment (P.E.D. %)			
a	1480*	1482	322-2 (92+)			
	1465*	1467	013-4 (83+)	013-5 (15+)		
	1460*	1461	013-2 (102+)			
	1455*	1454	013-7 (86+)	013-8 (16+)		
	1449*	1442	410-4 (96+)			
	1432*	1432	410-7 (96+)			
	1420*	1417	224-2 (80+)			
	1405	1400	322-5 (81+)	3224-S(12+)		
	1325*	1322	410-2 (103+)			
	1290	1292	322-6 (55+)	224-6 (19+)		
	1255	1251	224-5 (79+)			
	1218*	1219	013-5 (35+)	1322-S(21-)	224-6 (18+)	322-6 (11-)
	1180	1177	224-6 (32-)	013-5 (23+)	013-8 (19-)	
	1135	1148	013-8 (60+)	224-6 (13-)	322-6 (11+)	
	1122	1118	0132-S(47-)	1322-S(17+)	3224-S(17-)	
	1046	1049	3224-S(45+)	0132-S(34-)	322-4 (13+)	
	1005	1003	322-4 (32+)	224-4 (19-)	224-5 (8-)	0132-S(7+)
	964*	965	410-5 (83+)			
	959*	960	410-8 (48+)	1322-S(20+)	322-D (8-)	
	945*	954	410-8 (46+)	1322-S(21-)	322-D (8+)	
	792*	786	224-4 (58+)	1322-S(28+)		
	729	724	2410-S(86+)	2241-S(14-)		
	664	660	2241-S(78+)	2410-S(19+)		
	509	503	322-D (31-)	132-B (24-)	224-D (14+)	224-4 (8+)
	335	327	241-B (81-)	224-D (22+)	224-4 (10+)	
	335	322	132-B (59-)	322-D (22+)	224-D (18-)	
	228	227	0132-T(61-)	241-B (15-)	3224-T(14+)	
		193	0132-T(28+)	241-B (26-)	224-D (21-)	322-D (12-)
		157	2410-T(93+)			
		111	3224-T(56-)	1322-T(18-)		
		98	1322-T(55+)	224-D (18-)	2241-T(11+)	
		44	2241-T(80+)	3224-T(11+)		

Calculated frequencies higher than 2000 cm^{-1}

2989 2988 2964 2954 2953 2943 2904 2865 2857 2820

* Weight of the observed frequency is zero.

Reference

[1] IR.R. Y. Ogawa, M. Ohta, M. Sakakibara, H. Matsuura, I. Harada, and T. Shimanouchi, Bull. Chem. Soc. Jpn., **50**, 650 (1977).

No. 108
Molecule: 132241-GTG $CH_3OCH_2CH_2SCH_3$ **(gauche-trans-gauche form)**
Symmetry C_1 **Symmetry number** $\sigma = 1$

Sym. species	Observed frequency cm^{-1}	Calculated frequency cm^{-1}	Assignment (P.E.D. %)			
a	1480*	1480	322-2 (99+)			
	1465*	1467	013-4 (84+)	013-5 (15+)		
	1460*	1462	013-2 (103+)			
	1455*	1454	013-7 (86+)	013-8 (16+)		
	1449*	1442	410-4 (96+)			
	1432*	1432	410-7 (96+)			
	1420*	1417	224-2 (90+)			
	1373	1373	322-5 (90+)			
	1325*	1322	410-2 (102+)			
	1304	1300	322-6 (70+)	0132-S(5-)		
	1245*	1243	224-5 (76+)	224-6 (11-)		
	1218*	1234	224-6 (58+)	224-5 (19+)	322-4 (11+)	
	1196*	1195	013-5 (55+)	1322-S(17-)		
	1156*	1157	013-8 (80+)	013-7 (12-)		
	1098	1080	0132-S(50+)	1322-S(29-)	322-6 (10+)	
	1055*	1056	3224-S(70-)	322-D (7+)		
	980*	978	322-4 (38+)	224-4 (19+)	410-5 (17+)	1322-S(12-)
	964*	966	410-5 (74+)	322-4 (10-)		
	959*	958	410-8 (94+)			
	918	923	0132-S(43-)	1322-S(43-)		
	792*	792	224-4 (46+)	2241-S(22-)	322-4 (12-)	
	778	777	2241-S(44+)	224-4 (25+)	2410-S(8-)	
	703*	705	2410-S(93+)			
	468*	458	132-B (58-)	322-D (21+)	2241-S(13+)	
	363*	356	132-B (29+)	241-B (20-)	322-D (9+)	224-D (8+)
	303	304	241-B (67+)	322-D (23+)	224-D (20-)	224-4 (12-)
	228*	234	224-D (42+)	241-B (29+)	0132-T(14-)	
		178	0132-T(67+)	322-D (16-)	224-D (13+)	2410-T(11+)
		150	2410-T(83+)			
		118	1322-T(67+)	322-D (10+)		
		82	3224-T(60-)	2241-T(23+)		
		54	2241-T(64+)	3224-T(23+)	1322-T(11+)	

Calculated frequencies higher than 2000 cm^{-1}

2989 2988 2965 2954 2953 2942 2905 2865 2857 2820

* Weight of the observed frequency is zero.

Reference

[1] IR.R. Y. Ogawa, M. Ohta, M. Sakakibara, H. Matsuura, I. Harada, and T. Shimanouchi, Bull. Chem. Soc. Jpn., **50**, 650 (1977).

No. 109

Molecule: 132241-GTG′ $CH_3OCH_2CH_2SCH_3$ (gauche-trans-gauche′ form)

Symmetry C_1 Symmetry number $\sigma = 1$

Sym. species	Observed frequency cm^{-1}	Calculated frequency cm^{-1}	Assignment (P.E.D. %)			
a	1480*	1480	322-2 (99+)			
	1465*	1467	013-4 (84+)	013-5 (15+)		
	1460*	1462	013-2 (103+)			
	1455*	1454	013-7 (86+)	013-8 (16+)		
	1449*	1442	410-4 (96+)			
	1432*	1432	410-7 (96+)			
	1420*	1417	224-2 (90+)			
	1373	1373	322-5 (90+)			
	1325*	1322	410-2 (102+)			
	1304	1300	322-6 (70+)	0132-S(5-)		
	1245*	1242	224-5 (94+)	3224-S(10-)		
	1218*	1236	224-6 (68+)	322-4 (13+)		
	1196*	1195	013-5 (54+)	1322-S(17-)		
	1156*	1157	013-8 (80+)	013-7 (12-)		
	1098	1079	0132-S(51-)	1322-S(30+)	322-6 (10-)	013-5 (10+)
	1055*	1056	3224-S(71-)			
	980*	981	322-4 (38+)	224-4 (20+)	410-5 (14-)	1322-S(13-)
	964*	966	410-5 (76+)			
	959*	957	410-8 (92+)			
	918	922	0132-S(43-)	1322-S(43-)	322-4 (10-)	
	792*	791	224-4 (47+)	2241-S(20+)	322-4 (13-)	
	778	778	2241-S(46-)	224-4 (23+)	2410-S(8+)	
	703*	705	2410-S(93+)			
	468*	458	132-B (60-)	322-D (21+)	2241-S(13+)	
	363*	360	241-B (34+)	132-B (25-)	224-D (8-)	224-4 (8+)
	303	304	241-B (50+)	322-D (23+)	224-D (20-)	1322-T(12-)
	228*	227	224-D (43+)	241-B (32+)	0132-T(15-)	
		178	0132-T(64+)	322-D (17-)	224-D (13+)	2410-T(12-)
		150	2410-T(80+)	224-D (12+)		
		118	1322-T(68+)	2241-T(11-)		
		86	3224-T(69+)	2241-T(14-)		
		52	2241-T(70+)	3224-T(15+)	1322-T(12+)	

Calculated frequencies higher than 2000 cm^{-1}

2989 2988 2965 2954 2953 2942 2905 2865 2857 2820

* Weight of the observed frequency is zero.

Reference

[1] IR.R. Y. Ogawa, M. Ohta, M. Sakakibara, H. Matsuura, I. Harada, and T. Shimanouchi, Bull. Chem. Soc. Jpn., **50**, 650 (1977).